



ANL-WIS-MD-000009 REV 01

April 2004

# **Miscellaneous Waste-Form FEPs**

Prepared for: U.S. Department of Energy Office of Civilian Radioactive Waste Management Office of Repository Development 1551 Hillshire Drive Las Vegas, Nevada 89134-6321

Prepared by: Bechtel SAIC Company, LLC 1180 Town Center Drive Las Vegas, Nevada 89144

Under Contract Number DE-AC28-01RW12101

### DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, nor any of their contractors, subcontractors or their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or any third party's use or the results of such use of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof or its contractors or subcontractors. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

### **OCRWM**

## SCIENTIFIC ANALYSIS SIGNATURE PAGE/ CHANGE HISTORY

Page iii

1. Total Pages: 192

20 Apr 04

2. Scientific Analysis Title

Miscellaneous Waste-Form FEPs

3. DI (including Revision Number)

ANL-WIS-MD-000009 REV 01

4. Total Appendices 5. Number of Pages in Each Appendix

James A. Blink

Six (6)		<u>1-6; 11-4; 111-2; 1V-10; V-22, V1-4</u>	7
	Printed Name	Signature	Date
6. Originator	Thomas A. Thornton	SIGNATURE ON FILE	04/20/2008
7. Checker	Eric R. Siegmann Michael A. Jaeger	SIGNATURE ON FILE SIGNATURE ON FILE	4/20/2004
8. QER	Darrell K. Svalstad	SIGNATURE ON FILE	4/20/04

SIGNATURE ON FILE

### 11. Remarks

10. Responsible Manager

Thomas Thornton, Patrick Brady, James Cunnane, William Ebert, Paul Domski, Patricia Bernot, Yueting Chen, Christine Stockman, and Richard Aguilar contributed to this report.

Emma Thomas was responsible for the check and backcheck, while Eric Siegmann and Mike Jaeger were responsible for the final check and final backcheck. Howard Adkins was the Responsible Manager during development, but James Blink was the Responsible Manager during completion of the 2.14 review and final check.

	Change History
12. Revision/ICN No.	13. Description of Change
REV 00	Initial Issue.
	ICN changes: Ensured consistency with FEPs summary in Waste Form PMR. Made some editorial corrections and updated procedure references.
	Transferred the following three FEP discussions from this AMR (ANL-WIS-MD-000009) to the Clad Degradation FEPs AMR (ANL-WIS-MD-000008 REV 00 ICN 01):
REV 00 ICN 01	Volume Increase of Corrosion Products - YMP No. 2.1.09.03.0A
Idd v oo ich or	Gap and Grain release of Cs, I - YMP No. 2.1.02.07.00
	Rockfall (Large Block)- YMP No. 2.1.07.01.00
1	Transferred FEP discussion for mutations, YMP No. 2.1.13.03.00, from this AMR (ANL-WIS-MD-000009) to the Waste Form Colloid FEPs AMR (ANL-WIS-MD-000012).
REV 01	Complete revision to update the Waste-Form FEPs for the License Application.
10123 a	

## **CONTENTS**

				Page
1.	PI IR	POSE		1
1.	1.1		3	
	1.2		DENTIFICATION AND ANALYSIS - BACKGROUND	
	1.2	1.2.1	FEP Identification.	
		1.2.2	Integration of WF and WF Colloid FEP Screening into a FEP Database.	
2.	QUA	LITY A	SSURANCE	15
3.	USE	OF SOF	TWARE	17
4.	INPU			
	4.1	DIREC	CT INPUTS	19
	4.2	CRITE	RIA	
		4.2.1	Regulatory Basis for NRC Guidance	
	4.3	CODE	S AND STANDARDS	30
5.	ASS		DNS	
	5.1	GENE	RAL ASSUMPTIONS	
		5.1.1	Consistency with Design	
		5.1.2	Waste Type and Inventory	
	5.2		SPECIFIC ASSUMPTIONS	
		5.2.1	Igneous Intrusion Interacts with EBS Components (1.2.04.04.0A)	
		5.2.2	Waste Inventory (2.1.01.01.0A)	
		5.2.3	Interactions between Colocated Waste (2.1.01.02.0A)	32
		5.2.4	Interactions Between Codisposed Waste (2.1.01.02.0B)	32
		5.2.5	Heterogeneity of Waste Inventory (2.1.01.03.0A)	
		5.2.6	DSNF Degradation (Alteration, Dissolution, and Radionuclide Release) (2.1.02.01.0A)	
		5.2.7	CSNF Degradation (Alteration, Dissolution, and Radionuclide Release)	
			(2.1.02.02.0A)	32
		5.2.8	HLW Glass Degradation (Alteration, Dissolution, and Radionuclide	
			Release) (2.1.02.03.0A)	
		5.2.9	Alpha Recoil Enhances Dissolution (2.1.02.04.0A)	32
		5.2.10	HLW Glass Cracking (2.1.02.05.0A)	32
		5.2.11	HLW Glass Recrystallization (2.1.02.06.0A)	
		5.2.12	Radionuclide Release From Gap and Grain Boundaries (2.1.02.07.0A)	
		5.2.13	Pyrophoricity from DSNF (2.1.02.08.0A)	
		5.2.14	Chemical Effects of Void Space in the Waste Package (2.1.02.09.0A)	
		5.2.15	Organic/Cellulosic Materials in Waste (2.1.02.10.0A)	
		5.2.16	DSNF Cladding (2.1.02.25.0A)	
		5.2.17	Grouping of DSNF Waste Types into Categories (2.1.02.28.0A)	
		5.2.18	Flammable Gas Generation from DSNF (2.1.02.29.0A)	
		5.2.19	Internal Corrosion of Waste Packages Prior to Breach (2.1.03.06.0A)	34

# **CONTENTS (Continued)**

				Page
		5.2.20	Chemical Characteristics of Water in Waste Package (2.1.09.01.0B)	34
		5.2.21	Chemical Interaction with Corrosion Products (2.1.09.02.0A)	34
		5.2.22		
			Form and EBS (2.1.09.04.0A)	
		5.2.23	Reduction-Oxidation Potential in Waste Package (2.1.09.06.0A)	
		5.2.24	Reaction Kinetics in Waste Package (2.1.09.07.0A)	34
		5.2.25	Secondary Phase Effects on Dissolved Radionuclide Concentrations (2.1.09.10.0A)	
		5.2.26	Complexation in EBS (2.1.09.13.0A)	35
		5.2.27	Formation of True (Intrinsic) Colloids in EBS (2.1.09.15.0A)	35
		5.2.28	Formation of Pseudo-Colloids (Natural) in EBS (2.1.09.16.0A)	
			Formation of Pseudo-Colloids (Corrosion Product) in EBS (2.1.09.17.0A	
		5.2.30	Formation of Microbial Colloids in EBS (2.1.09.18.0A)	
		5.2.31	Stability of Colloids in EBS (2.1.09.23.0A)	35
		5.2.32	Formation of Colloids (Waste-Form) by Coprecipitation in EBS	
			(2.1.09.25.0A)	35
		5.2.33	,	35
		5.2.34	Thermal Effects on Chemistry and Microbial Activity in the EBS (2.1.11.08.0A)	36
		5 2 35	Thermally Driven Flow (Convection) in the EBS (2.1.11.09.0B)	
		5.2.36		50
		3.2.30	(2.1.12.04.0A)	36
		5.2.37		
		5.2.38	Radiolysis (2.1.13.01.0A)	
		5.2.39	Radiation Damage in EBS (2.1.13.02.0A)	
		5.2.40	Chemistry of Water Flowing into Waste Package (2.2.08.12.0B)	
		5.2.41	Radioactive Decay and In-Growth (3.1.01.01.0A)	
		0.2	Thursday and in Growth (5.1.01.011)	
6.	SCIE	NTIFIC	ANALYSIS DISCUSSION	37
	6.1		DACHES	
	6.2	WAST	E-FORM FEPS SCREENING AND ANALYSES	52
		6.2.1	Igneous Intrusion Interacts with EBS Components	
		6.2.2	Waste Inventory	55
		6.2.3	Interactions between Colocated Waste	56
		6.2.4	Interactions Between Codisposed Waste	58
		6.2.5	Heterogeneity of Waste Inventory	
		6.2.6	DSNF Degradation (Alteration, Dissolution, and Radionuclide Release).	
		6.2.7	CSNF Degradation (Alteration, Dissolution, and Radionuclide Release)	63
		6.2.8	HLW Glass Degradation (Alteration, Dissolution, and Radionuclide	
			Release)	65
		6.2.9	Alpha Recoil Enhances Dissolution	
		6.2.10	HLW Glass Cracking	
		6.2.11	HLW Glass Recrystallization	
		6.2.12	Radionuclide Release from Gap and Grain Boundaries	73

# **CONTENTS (Continued)**

			rage
	6.2.13	Pyrophoricity from DSNF	74
	6.2.14	Chemical Effects of Void Space in Waste Package	
		Organic/Cellulosic Materials in Waste	
	6.2.16	DSNF Cladding	
	6.2.17	Grouping of DSNF Waste Types into Categories	80
	6.2.18	Flammable Gas Generation from DSNF	81
	6.2.19	Internal Corrosion of Waste Packages Prior To Breach	84
	6.2.20	Chemical Characteristics of Water in Waste Package	85
	6.2.21		
	6.2.22	Radionuclide Solubility, Solubility Limits, and Speciation in the Waste Form and EBS	
	6.2.23	Reduction-Oxidation Potential in Waste Package	89
	6.2.24	Reaction Kinetics in Waste Package	
	6.2.25	Secondary Phase Effects on Dissolved Radionuclide Concentrations	92
	6.2.26	Complexation in EBS	94
	6.2.27	Formation of True (Intrinsic) Colloids in EBS	95
	6.2.28	Formation of Pseudo-Colloids (Natural) in EBS	
	6.2.29	Formation of Pseudocolloids (Corrosion Product) in EBS	98
	6.2.30	Formation of Microbial Colloids in EBS	
	6.2.31	Stability of Colloids in EBS	
	6.2.32	Formation of Colloids (Waste-Form) by Coprecipitation in EBS	
	6.2.33	Exothermic Reactions in EBS	
	6.2.34	Thermal Effects on Chemistry and Microbial Activity in the EBS	
	6.2.35	Thermally Driven Flow (Convection) in the EBS	
	6.2.36	Gas Generation (CO <sub>2</sub> , CH <sub>4</sub> , H <sub>2</sub> S) From Microbial Degradation	106
	6.2.37	Effects of Radioactive Gases in EBS	
	6.2.38	Radiolysis	
	6.2.39	Radiation Damage in EBS	
	6.2.40	Chemistry of Water Flowing into Waste Package	
	6.2.41	Radioactive Decay and In-growth	114
7.	CONCLUSIO	ONS	117
8.		O REFERENCES	
		MENTS CITED	
	8.2 CODE	S, STANDARDS, REGULATIONS, AND PROCEDURES	128
	8.3 SOUR	CE DATA, LISTED BY DATA TRACKING NUMBER	129
9.	ATTACHME	NTS	131

### **FIGURES**

		Page
1.	Illustration of the FEP Screening Process	4
2.	Comparison of Dissolution Rates for High-Level Radioactive Waste, Metallic Carbide, and Ceramic Spent Nuclear Fuel	
	TABLES	
		Page
1.2-1.	Waste-Form and Waste-Form Colloid FEPs for TSPA-LA	5
4-1.	Direct Inputs to Waste-Form FEPs Screening Decision to Include	20
6-1.	Supporting Information for Waste-Form FEPs Disposition	
6.2-1.	Alpha Recoil Enhanced (From $\alpha$ and $\alpha$ -Recoil Atom) Dissolution Rates Due to the	
	Major Mass-Based Constituents of SNF and HLW to be Disposed of in the Yucca	
	Mountain Repository	70
9-1.	List of Attachments	131

#### **ACRONYMS**

ANL Argonne National Laboratory

AR analysis report

ATM approved testing material

BWR boiling water reactor

COM Center of Mass (frame of reference)
CSNF commercial spent nuclear fuel

DOE U.S. Department of Energy DHLWG defense high-level waste glass DSNF DOE-owned spent nuclear fuel

EBS Engineered Barrier System

Eh redox potential

EIS Environmental Impact Statement

EPA U.S. Environmental Protection Agency

FEPs features, events, and processes

HLW high-level radioactive waste

INEEL Idaho National Engineering and Environmental Laboratory

IPCM In-Package Chemistry Model

KE kinetic energy

MCO multi-canister overpack

MOX mixed oxide MR model report

MTHM metric tons heavy metal

NRC U.S. Nuclear Regulatory Commission

ORD Office of Repository Development

pH negative logarithm to the base 10 of the effective hydrogen-ion concentration

PWR pressurized water reactor

RCRA Resource Conservation and Recovery Act

SF spontaneous fission SNF spent nuclear fuel

### **ACRONYMS (Continued)**

TRIGA training, research, isotopics General Atomics (U-Zr-Hx)

TSPA Total System Performance Assessment

TSPA-LA Total System Performance Assessment-License Application
TSPA-SR Total System Performance Assessment-Site Recommendation
TSPA-VA Total System Performance Assessment-Viability Assessment

WF waste form

WPE waste package equivalent

YMP Yucca Mountain Project

### 1. PURPOSE

This scientific analysis report focuses on Waste-Form and Waste-Form Colloid features, events, and processes (FEPs) to be considered in the TSPA model for the License Application.

The U.S. Department of Energy (DOE) must provide a reasonable assurance that the performance objectives for the Office of Repository Development (ORD) radioactive waste repository described in 10 CFR 63.113 [DIRS 156605] can be achieved for a 10,000-year postclosure period. The requirements for the postclosure performance assessment to provide this assurance are given in 10 CFR 63.114 [DIRS 156605]. The performance assessment is an analysis that (10 CFR 63.2 [DIRS 156605]):

- 1. Identifies the features, events, processes (except human intrusion), and sequences of events and processes (except human intrusion) that might affect the Yucca Mountain disposal system and their probabilities of occurring during 10,000 years after disposal
- 2. Examines the effects of those features, events, and processes and sequences of events and processes upon the performance of the Yucca Mountain disposal system
- 3. Estimates the dose incurred by the reasonably maximally exposed individual, including the associated uncertainties, as a result of releases caused by all significant features, events, processes, and sequences of events and processes, weighted by their probability of occurrence.

To demonstrate that regulatory-specified performance objectives of 10 CFR 63.113 [DIRS 156605] can be achieved for a 10,000-year postclosure period, the ORD is implementing a FEP analysis and scenario-development methodology based on the work of Cranwell et al. (1990 [DIRS 101234]). The methodology, incorporated into a total system performance assessment (TSPA), provides a systematic approach for considering, as completely as practicable, the possible future states of a repository system. The TSPA seeks to include all possible future states using a finite set of scenario classes. A scenario is a well-defined, connected sequence of FEPs that outlines a possible future condition of the proposed repository system. A scenario class is a set of related scenarios sharing sufficient similarities that can usefully be aggregated for the purposes of screening or analysis. The objective of FEP analysis and scenario development is to define a limited set of scenario classes and scenarios that can reasonably be analyzed quantitatively while still maintaining comprehensive coverage of the range of possible future states of the disposal system.

FEPs are a fundamental aspect of a performance assessment, where (NRC 2003 [DIRS 163274], Section 3):

- 1. A feature is an object, structure, or condition with a potential to affect disposal system performance.
- 2. An event is a natural or human-caused phenomenon with a potential to affect disposal system performance and that occurs during an interval that is short compared to the period of performance.

3. A process is a natural or human-caused phenomenon with a potential to affect disposal system performance and that operates during all or a significant part of the period of performance.

The identification of FEPs that are relevant to the functioning of the disposal system conceptually produces the initial domain or parameter space of the disposal system model. A screening process omits those portions of the domain that are not pertinent. The formal and defensible selection of the pertinent domain of FEPs when developing the conceptual model of the disposal system is one aspect that sets performance assessment apart from typical scientific or engineering analyses. Because of the nature of FEP screening and model development, several iterations of the performance assessment process are potentially necessary to eliminate those FEPs of negligible influence (excluded FEPs) and to improve the modeling of those retained FEPs (included FEPs).

### 1.1 SCOPE

This scientific analysis report is governed by *Technical Work Plan for Waste Form Degradation Modeling, Testing, and Analyses in Support of LA* (BSC 2004 [DIRS 167796]) and Work Package AWFM01, WF Modeling and Analysis for LA.

This report addresses the waste form (WF) and WF colloid FEPs, as extracted and updated from the LA FEP list (DTN: MO0307SEPFEPS4.000 [DIRS 164527]). The scope of this report is two-fold:

- 1. It summarizes the TSPA-LA disposition (i.e., how the FEP is implemented) for the WF and WF colloid FEPs that are included in the TSPA-LA analysis model, and relates the FEPs to the scientific analysis reports or model reports in which these dispositions are developed and documented.
- 2. It documents the screening argument (i.e., technical basis and rationale) for the WF and WF colloid FEPs that are excluded from the TSPA-LA analysis based on criteria identified in Section 4.2 of this report.

### 1.2 FEPS IDENTIFICATION AND ANALYSIS - BACKGROUND

### 1.2.1 FEP Identification

The development of a comprehensive list of FEPs potentially relevant to post-closure performance of the Yucca Mountain repository is an ongoing, iterative process based on site-specific information, design, and regulations. The first step of the FEP analysis process is the identification of FEPs potentially relevant to the performance of the potential Yucca Mountain repository. An initial list of FEPs relevant to Yucca Mountain was developed from a comprehensive list of FEPs from radioactive waste disposal programs in other countries (BSC 2001 [DIRS 154365], Section 2.1) and was supplemented with additional YMP-specific FEPs from project literature, technical workshops, and reviews (BSC 2001 [DIRS 154365], Sections 2.2 through 2.4). The initial FEP list contained 328 FEPs, of which 176 were "included" in TSPA-SR models (CRWMS M&O 2000 [DIRS 153246], Tables B-9 through B-17). Although *Total System Performance Assessment for the Site Recommendation* (CRWMS

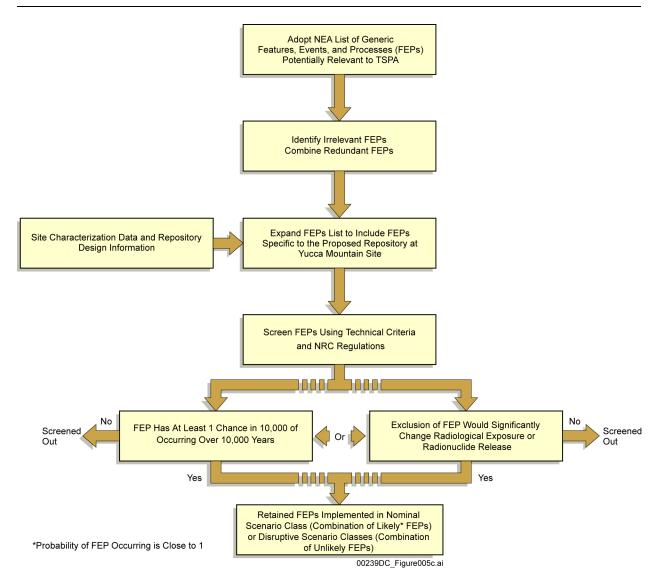
M&O 2000 [DIRS 153246]) was cancelled along with other TSPA-SR process-level reports, it adequately explained the initial FEPs listing.

For TSPA-LA, a reorganization and re-evaluation of the FEP list was undertaken in accordance with *The Enhanced Plan for Features, Events, and Processes (FEPs) at Yucca Mountain* (BSC 2002 [DIRS 158966], Section 3.2) and *KTI Letter Report, Response to Additional Information Needs on TSPAI 2.05 and TSPAI 2.06* (Freeze 2003 [DIRS 165394]). The FEPs were then assigned to one or more FEP analysis reports, each of which addresses a specific technical area. In some cases, where a FEP covered multiple technical areas, it was shared by multiple FEP analysis reports. In these cases, a single FEP analysis report may provide only a partial technical basis for the screening of the FEP. The full technical basis for these shared FEPs is addressed collectively by all of the sharing FEP analysis reports.

The reorganization and reevaluation resulted in a preliminary list of 47 WF and WF colloid FEPs as extracted from the LA FEP list (DTN: MO0307SEPFEPS4.000 [DIRS 164527]. Subsequent evaluation of the scope of these WF FEPs resulted in 7 FEPs being reassigned from this report to other FEP analysis reports and 1 FEP being reassigned from other FEP analysis reports to this report. The resulting 41 WF and WF colloid FEPs that are addressed in this report are listed in Table 1.2-1. Additional WF FEPs (clad related) are addressed in *Clad Degradation – FEPs Screening Arguments* (BSC 2003 [DIRS 165057]).

The second step of the FEP analysis process is the screening of potentially relevant FEPs based on the criteria identified in Section 4.2.1. A schematic of the FEP identification and screening process is given in Figure 1. Although shown as sequential activities, iteration occurs as new information becomes available that might result in new FEPs and/or changes to the technical bases for screening.

Table 1.2-1 provides the FEP number, name, description, and screening decision for each of the 41 WF FEPs. Note that the screening decisions are based on information documented in Section 6.2 of this report. Note also that FEP names and descriptions have been revised from the LA FEP list (DTN: MO0307SEPFEPS4.000 [DIRS 164527]) for FEPs 2.1.09.06.0A and 2.1.09.07.0A to accommodate a splitting of the FEPs and that FEP descriptions have been modified for FEPs 1.2.04.04.0A, 2.1.01.01.0A, 2.1.01.03.0A, 2.1.02.04.0A, 2.1.02.06.0A, 2.1.02.07.0A, 2.1.02.29.0A, 2.1.09.02.0A, 2.1.09.16.0A, 2.1.09.17.0A, and 2.1.13.02.0A to correct minor errors. Table 1.2-1 also identifies shared FEPs and, for included FEPs, it identifies the supporting model and analysis reports that further describe the implementation of the FEP.



Source: BSC 2003 [DIRS 166296], Figure 3.2-2

Figure 1. Illustration of the FEP Screening Process

### 1.2.2 Integration of WF and WF Colloid FEP Screening into a FEP Database

Under a separate scope of work, the Office of Repository Development FEP team is constructing a FEP database (BSC 2004 [DIRS 168024]) and the associated LA FEP list (DTN: MO0307SEPFEPS4.000 [DIRS 164527]) to assist the Yucca Mountain Project during the license review process. Fields within each entry provide a unique identification number, a description of the FEP, its origin, and mapping to related FEPs and to the assigned scientific analysis reports or model reports. Fields also provide summaries of the screening arguments with references to supporting documentation, and, for all included FEPs, statements of disposition of the FEP within the TSPA. The FEP discussions in this scientific analysis report provide summaries and dispositions for the waste-form FEPs to be included in the FEP database.

Table 1.2-1. Waste-Form and Waste-Form Colloid FEPs for TSPA-LA

LA FEP Number	FEP Name	LA FEP Description	Supporting Reports for Included FEPs	Shared FEP	LA Screening Decision
1.2.04.04.0A	Igneous intrusion interacts with EBS components	An igneous intrusion in the form of a dike occurs through the repository, intersecting the repository drifts. Magma, pyroclastics, and volcanic gases enter the drift and interact with the EBS components including the drip shields, the waste packages, pallet, and invert. This leads to accelerated drip shield and waste package failure (e.g. attack by magmatic volatiles, damage by flowing or fragmented magma, thermal effects) and dissolution or volatilization of waste.	BSC 2004 [DIRS 167654]	DE	Included
2.1.01.0A	Waste inventory	The waste inventory includes all potential sources of radiotoxicity and chemical toxicity. It consists of the radionuclide inventory (typically in units of curies), by specific isotope, of anticipated radionuclides in the waste, and the non-radionuclide inventory (typically in units of density or concentration) that consists of both physical, e.g., CSNF, DNSF, and HLW, and chemical waste constituents. The radionuclide composition of the waste will vary due to initial enrichment, burnup, the number of fuel assemblies per container, and the decay time subsequent to discharge of the fuel from the reactor.  Also consider that the fuel types, matrices, radionuclide mixes, and non-radionuclide inventories in DSNF and HLW may differ from CSNF. Additional waste types should be considered if they are proposed for disposal at Yucca Mountain.	BSC 2003 [DIRS 161961]	N/A	Included
2.1.01.02.0A	Interactions between colocated waste	Colocation refers to the disposal of CSNF, DSNF, HLW, and possibly other wastes in close proximity within the repository. Colocation might affect thermal outputs, chemical interactions, or radionuclide mobilization.	N/A	N/A	Excluded (low consequence)
2.1.01.02.0B	Interactions between codisposed waste	Codisposal refers to the disposal of different waste types within the same waste package. Codisposal might affect chemical interactions or radionuclide mobilization. At Yucca Mountain, the DSNF will be combined with HLW canisters within a waste package. This codisposal with HLW within a waste package is unique to the DSNF and does not apply to the CSNF placement within waste packages.  The DSNF will be contained within canisters that will be placed within the waste packages. The use of canisters within the waste packages. The use of canisters within the waste packages. Also, some DSNF waste packages may contain only DSNF canisters, while others may contain both DSNF and HLW canisters.	BSC 2003 [DIRS 161962] BSC 2003 [DIRS 163693] BSC 2004 [DIRS 167619]	A/A	Included

Table 1.2-1. Waste-Form and Waste-Form Colloid FEPs for TSPA-LA (Continued)

3
nuclear fuel (DSNF), and high-level waste (HLW) shipped to the repository may contain quantities of radionuclides that vary from waste package to waste package, fuel assembly to fuel assembly, and from canister to canister. The composition of each of these waste forms may vary due to initial uranium enrichment, possible plutonium enrichment, and burnup of the fuel, among other factors. The physical state within the waste form may also vary. For example, damaged fuel pellets or extremely high-burnup fuels may have greater surface area exposed to any water penetrating a waste package than undamaged, low-burnup spent fuel. Given these potential differences in isotopic composition and physical condition, the mass of radionuclides available for transport may vary significantly among waste packages.  The different physical (structure, geometry), chemical, and radiological properties of the many forms of CSNF, DSNF, and HLW could result in differences in the corrosion and alteration rates of the waste package composition. This could affect repository chemistry, breach times, dissolution rates, and availability of radionuclides for transport.
DSNF to be disposed of in Yucca Mountain has a variety of fuel types that include metallic uranium fuels; oxide and MOX fuels; Three Mile Island rubble; and heterogeneous fuels such as UAIx, U-ZrHx, and graphite fuels. In general, the composition and structure of these spent fuels are significantly different from the commercial spent nuclear fuel (CSNF), and degradation, alteration, and dissolution may be different from the CSNF degradation.  Processes to be considered in this FEP include alteration and dissolution of the various DSNF waste forms, phase separation, oxidation of spent fuels, selective leaching, and the effects of the high-intentity can (HC) on DSNF degradation.

Table 1.2-1. Waste-Form and Waste-Form Colloid FEPs for TSPA-LA (Continued)

LA FEP Number	FEP Name	LA FEP Description	Supporting Reports for Included FEPs	Shared FEP	LA Screening Decision
2.1.02.02.0A	CSNF degradation (alteration, dissolution, and radionuclide release)	Alteration of the original mineralogy of the commercial spent nuclear fuel (CSNF) (under wet or dry conditions) and dissolution of the uranium-oxide matrix can influence the mobilization of radionuclides. The degradation of UO <sub>2</sub> could be affected by a number of variables, such as surface area, burnup, temperature, overall solution electrochemical potential (Eh), pH, and especially solutions containing significant concentrations of calcium, sodium, carbonate and silicate ions, as well as availability of organic complexing materials. In turn, these water properties are affected by the alteration of the cladding and matrix.	BSC 2004 [DIRS 167321]	N/A	Included
2.1.02.03.0A	HLW glass degradation (alteration, dissolution, and radionuclide release)	Glass waste forms are thermodynamically unstable over long time periods, and will alter on contact with water. Radionuclides can be mobilized from the glass waste by a variety of processes, including degradation and alteration of the glass, phase separation, congruent dissolution, precipitation of silicates, coprecipitation of other minerals including iron corrosion products, and selective leaching.	BSC 2004 [DIRS 167619]	N/A	Included
2.1.02.04.0A	Alpha recoil enhances dissolution	During decay of certain radionuclides, alpha particles may be emitted with sufficiently high energies that the daughter nuclide recoils appreciably to conserve system momentum. A potential result of recoil is that certain radionuclides, such as <sup>234</sup> U, exhibit substantially greater dissolution rates (with the same solubility limits) and can be transported preferentially.	N/A	N/A	Excluded (low consequence)
2.1.02.05.0A	HLW glass cracking	Cracking of the HLW glass on cooling and during handling means that the surface area of the glass is greater than the surface area of a monolithic block. The increase in the surface area could affect the rate of glass alteration and radionuclide dissolution.	BSC 2004 [DIRS 167619]	N/A	Included
2.1.02.06.0A	HLW glass recrystallizati on	HLW glass recrystallization could occur and would lead to a less corrosion-resistant waste form. Recrystallization is a slow process and typically occurs only if a high glass temperature is maintained over a prolonged period.	BSC 2004 [DIRS 167619]	۲ ک	Included

Table 1.2-1. Waste-Form and Waste-Form Colloid FEPs for TSPA-LA (Continued)

LA FEP Number	FEP Name	LA FEP Description	Supporting Reports for Included FEPs	Shared FEP	LA Screening Decision
2.1.02.07.0A	Radionuclide release from gap and grain boundaries	While in the reactor at the high temperatures, radionuclides such as I and Cs may migrate and preferentially accumulate in cracks in the fuel matrix, grain boundaries of the $\mathrm{UO}_2$ , and in the gap between the fuel and cladding. If the waste package fails and the cladding perforates, the release rate of this fraction of the radionuclides could be rapid. In addition, reactions between materials within the spent fuel assembly or waste package infill such as I and Pb may affect this process.	BSC 2004 [DIRS 167321]	Ϋ́Α V	Included
2.1.02.08.0A	Pyrophoricity from DSNF	DSNF can contain pyrophoric material. Pyrophoric material could ignite and produce an adverse effect on repository performance. Pyrophoric events could affect the thermal behavior of the system and could contribute to degradation of the waste package, waste form, and cladding.	N/A	N/A	Excluded (low consequence)
2.1.02.09.0A	Chemical effects of void space in waste package	If waste packages and/or DSNF canisters are not completely filled, then the unfilled inert-gas or air-filled volume could influence water-chemistry calculations.	BSC 2003 [DIRS 161962]	N/A	Included
2.1.02.10.0A	Organic / cellulosic materials in waste	Degradation of cellulose in the waste could affect the long-term performance of the disposal system.	N/A	N/A	Excluded (low consequence)
2.1.02.25.0A	DSNF cladding	DSNF to be disposed of in Yucca Mountain has a variety of fuel types that may not be similar to the CSNF to be disposed. Some of the fuel types may have initial cladding-degradation characteristics that are different from those for the CSNF.  Therefore, the effectiveness of DSNF cladding as a barrier to radionuclide mobilization might be different from CSNF. This FEP addresses all types of DSNF cladding except Naval SNF cladding.	N/A	¥,	Excluded (low consequence)
2.1.02.28.0A	Grouping of DSNF waste types into categories	Several hundred distinct types of DOE-owned SNF (DSNF) may potentially be stored at YMP. These represent many more types than can viably be examined for their individual effect on the repository. A limited number of representative or bounding degradation models must be selected and/or abstracted. As a result, the effects on repository performance of the details related to the many distinct types of DSNF can not be evaluated.	BSC 2003 [DIRS 163693]	¥ Z	Included

Table 1.2-1. Waste-Form and Waste-Form Colloid FEPs for TSPA-LA (Continued)

LA FEP Number	FEP Name	LA FEP Description	Supporting Reports for Included FEPs	Shared FEP	LA Screening Decision
2.1.02.29.0A	Flammable gas generation from DSNF	DOE-owned Spent Nuclear Fuel (DSNF) to be disposed of in Yucca Mountain will have a small percent of carbide fuel. When carbide is exposed to water, flammable gases such as methane and its minor constituents ethane, ethylene, and acetylene (referred as ethyne by the International Union of Pure and Applied Chemistry) are generated. If these gases ignite, localized increases in temperature can occur, which might affect fuel degradation. The area around the ignition point may be mechanically and/or thermally perturbed, which could affect waste container or host-rock properties in the area of the EBS.	N/A	N/A	(low consequence)
2.1.03.06.0A	Internal corrosion of waste packages prior to breach	Aggressive chemical conditions within the waste package could contribute to corrosion from the inside out. Effects of different waste forms, including CSNF and DSNF, are considered in this FEP.	N/A	WP	Excluded (low consequence)
2.1.09.01.0B	Chemical characteristi cs of water in waste package	Chemical characteristics of the water in the waste packages (pH and dissolved species) may be affected by interactions with materials or steel used in the waste packages or waste forms and by the inflowing water from the drifts and near-field host rock.  The in-package chemistry, in turn may influence dissolution and transport as contaminants move through the waste, EBS, and down into the unsaturated zone.	BSC 2003 [DIRS 161962]	N/A	Included
2.1.09.02.0A	Chemical interaction with corrosion products	Corrosion products produced during degradation of the waste form, metallic portions of the waste package, and metals in the drift (rock bolts, steel in invert, gantry rails) may affect the mobilization and transport of radionuclides. Corrosion products may facilitate sorption/desorption and coprecipitation/dissolution processes. Corrosion products may form a "rind" around the fuel that could (1) restrict the availability of water for dissolution of radionuclides or (2) inhibit advective or diffusive transport of water and radionuclides from the waste form to the EBS. Corrosion products also have the potential to retard the transport of radionuclides to the EBS. Finally, corrosion products may alter the local chemistry, possibly enhancing dissolution rates for specific waste forms, or altering radionuclide solubility.	BSC 2003 [DIRS 161962] BSC 2004 [DIRS 167619] BSC 2003 [DIRS 166845]	EBS	Included

Table 1.2-1. Waste-Form and Waste-Form Colloid FEPs for TSPA-LA (Continued)

LA FEP Number	FEP Name	LA FEP Description	Supporting Reports for Included FEPs	Shared FEP	LA Screening Decision
2.1.09.04.0A	Radionuclide solubility, solubility limits, and speciation in the waste form and EBS	Degradation of the waste form will mobilize radionuclides in the aqueous phase. Factors to be considered in this FEP include the initial radionuclide inventory, justification of the limited inventory included in evaluations of aqueous concentrations, and the solubility limits for those radionuclides.	BSC 2003 [DIRS 163152]	<b>∀</b> /∀	Included
2.1.09.06.0A	Reduction- oxidation potential in waste package	The redox potential in the waste package influences the oxidation of waste-form materials and the in-package solubility of radionuclide species. Local variations in the in-package redox potential can occur.	BSC 2003 [DIRS 161962]	N/A	Included
2.1.09.07.0A	Reaction kinetics in waste package	Chemical reactions, such as radionuclide dissolution/ precipitation reactions and reactions controlling the reduction- oxidation state, may not be at equilibrium within the waste package.	BSC 2003 [DIRS 161962]	N/A	Included
2.1.09.10.0A	Secondary phase effects on dissolved radionuclide concentratio ns	Inclusion of radionuclides in secondary uranium mineral phases, such as neptunium in schoepite and uranium silicates, could affect radionuclide concentrations in water in contact with the waste form. During radionuclide alteration, the radionuclides could be chemically bound to immobile compounds and result in a reduction of available radionuclides for mobilization.	N/A	Z/A	Excluded (low consequence)
2.1.09.13.0A	Complexatio n in EBS	The presence of organic complexants in water in the EBS could augment radionuclide transport by providing a transport mechanism in addition to simple diffusion and advection of dissolved material. Organic complexants may include materials found in natural groundwater such as humates and fulvates, or materials introduced with the waste or engineered materials.	N/A	N/A	Excluded (low consequence)
2.1.09.15.0A	Formation of true (intrinsic) colloids in EBS	True colloids are colloidal-sized assemblages (between approximately 1 nanometer and 1 micrometer in diameter) consisting of hydrolyzed and polymerized radionuclides. They may form in the waste package and EBS during waste -form degradation and radionuclide transport. True colloids are also called primary colloids, real colloids, Type I colloids, Eigenkolloide, and intrinsic colloids (or actinide intrinsic colloids, for those including actinide elements).	N/A	₹ 2	Excluded (low consequence)

Table 1.2-1. Waste-Form and Waste-Form Colloid FEPs for TSPA-LA (Continued)

LA FEP Number	FEP Name	LA FEP Description	Supporting Reports for Included FEPs	Shared FEP	LA Screening Decision
2.1.09.16.0A	Formation of pseudo-colloids (natural) in EBS	Pseudo-colloids are colloidal-sized assemblages (between approximately 1 nanometer and 1 micrometer in diameter) of nonradioactive material that have radionuclides bound or sorbed to them. Natural pseudo-colloids include microbial colloids, mineral fragments (clay, silica, iron oxyhydroxides), and humic and fulvic acids. This FEP addresses radionuclide-bearing pseudo-colloids formed from host-rock materials and all interactions of the waste and EBS with the host rock environment except corrosion.	BSC 2003 [DIRS 166845]	Υ/A	Included
2.1.09.17.0A	Formation of pseudo-colloids (corrosion product) in EBS	Pseudo-colloids are colloidal-sized assemblages (between approximately 1 nanometer and 1 micrometer in diameter) of nonradioactive material that have radionuclides bound or sorbed to them. Corrosion product pseudo-colloids include iron oxyhydroxides from corrosion and degradation of the metals in the EBS and silica from degradation of cementitious materials.	BSC 2003 [DIRS 166845]	N/A	Included
2.1.09.18.0A	Formation of microbial colloids in EBS	This FEP addresses the formation and transport of microbial colloids in the waste and EBS.	N/A	N/A	Excluded (low consequence)
2.1.09.23.0A	Stability of colloids in EBS	For radionuclide-bearing colloids to affect repository performance, the colloids in the dispersion must remain suspended, that is, be stable, for time scales that are long relative to time required for groundwater travel. Further, they must carry significant concentrations of radionuclides. The stability of smectite colloids, which is applicable for YMP groundwater colloids and waste-form colloids, is determined primarily by ionic strength but also to an extent by pH. The stability of iron oxyhydroxide colloids, which is applicable to corrosion-product colloids, is determined by both ionic strength and pH.	BSC 2003 [DIRS 166845]	N/A	Included
2.1.09.25.0A	Formation of colloids (waste form) by coprecipitati on in the EBS	Dissolved radionuclides and other ions may coprecipitate to form colloids. Coprecipitates may consist of radionuclides bound in the crystal lattice of a dominating mineral phase or may consist of radionuclides engulfed by a dominating mineral phase.	BSC 2003 [DIRS 166845]	Ϋ́,	Included

Table 1.2-1. Waste-Form and Waste-Form Colloid FEPs for TSPA-LA (Continued)

LA FEP Number	FEP Name	LA FEP Description	Supporting Reports for Included FEPs	Shared FEP	LA Screening Decision
2.1.11.03.0A	Exothermic reactions in the EBS	Exothermic reactions liberate heat and will alter the temperature of the disposal system and affect the properties of the repository and surrounding materials. Oxidation of uranium metal fuels such as represented by N-Reactor fuels is one example of a possible exothermic reaction. Hydration of concrete used in the underground environment is another example of a possible exothermic reaction in the EBS.	NA	EBS	Excluded (low consequence)
2.1.11.08.0A	Thermal effects on chemistry and microbial activity in the EBS	Temperature changes may affect chemical and microbial processes in the waste and EBS.	BSC 2003 [DIRS 161962]	EBS	Included
2.1.11.09.0B	Thermally- driven flow (convection) in the EBS	Temperature differentials may result in convective flow in the EBS. Convective flow within the waste and EBS could influence in-package chemistry.	N/A	EBS	Excluded (low consequence)
2.1.12.04.0A	Gas generation (CO <sub>2</sub> , CH <sub>4</sub> , H <sub>2</sub> S) from microbial degradation	Microbes are known to produce inorganic acids, methane, organic byproducts, carbon dioxide, and other chemical species that could change the longevity of materials in the repository and the transport of radionuclides from the near field. The rate of microbial gas production will depend on the nature of the microbial populations established, the prevailing conditions (temperature, pressure, geochemical conditions), and the organic or inorganic substrates present. Initial analysis indicates the most important source of nutrient in the YMP repository will be metals. Other possible nutrients include cellulosic material, plastics, and synthetic materials. Minimal amounts of organics are mandated by regulation.	N/A	EBS	(low consequence)
2.1.12.07.0A	Effects of radioactive gases in EBS	Radioactive gases may exist or be produced in the repository. These gases may subsequently escape from the repository. Typical radioactive gases include $^{14}$ C (in $^{14}$ CO $_2$ and $^{14}$ CH $_4$ ) produced during microbial degradation, tritium, fission gases (Ar, Xe, Kr), and radon.	N/A	EBS	Excluded (low consequence)

Table 1.2-1. Waste-Form and Waste-Form Colloid FEPs for TSPA-LA (Continued)

LA FEP Number	FEP Name	LA FEP Description	Supporting Reports for Included FEPs	Shared FEP	LA Screening Decision
2.1.13.01.0A	Radiolysis	Alpha, beta, gamma, and neutron irradiation of water can cause dissociation of molecules, leading to gas production and changes in chemical conditions (Eh, pH, concentration of reactive radicals).	N/A	WP	Excluded (low consequence)
2.1.13.02.0A	Radiation damage in EBS	Radiolysis due to the alpha, beta, gamma-ray, and neutron irradiation of water could result in the enhancement for the movement of the radionuclides from the surface of a degraded waste form into groundwater flow. When radionuclides decay, the emitted high-energy particle could result in the production of radicals in the water or air surrounding the spent nuclear fuel. If these radicals migrate (diffuse) to the surface of the fuel (UO <sub>2</sub> ). This effect would increase the dissolution rate for radionuclides from the fuel material (fuel meat) into the groundwater flow. Strong radiation fields could lead to radiation damage to the waste forms and containers (CSNF, DSNF, DHLW), drip shield, seals and surrounding rock.	N/A	EBS	(low consequence)
2.2.08.12.0B	Chemistry of water flowing into the waste package	Inflowing water chemistry may be used in analysis or modeling that requires initial water chemistry in the waste package.	BSC 2003 [DIRS 161962] (FEP 2.2.08.12.0B is not in the included FEP table in the currently controlled REV 02 of this model report. It will be added to the next ICN/REV of the model report.	N/A	Included
3.1.01.0A	Radioactive decay and in-growth	Radioactivity is the spontaneous disintegration of an unstable atomic nucleus that results in the emission of subatomic particles. Radioactive isotopes are known as radionuclides. Radioactive decay of the fuel in the repository changes the radionuclide content in the fuel with time and generates heat. Radionuclide quantities in the system at any time are the result of the radioactive decay and the growth of daughter products as a consequence of that decay (i.e., ingrowth). Over a 10,000-year performance period, these processes will produce daughter products that need to be considered in order to adequately evaluate the release and transport of radionuclides to the accessible environment.	BSC 2003 [DIRS 161961]	SZ UZ BIO	Included

13

### 2. QUALITY ASSURANCE

The scientific analysis documented in this report was performed in accordance with AP-SIII.9Q, Scientific Analyses and evaluated in accordance with AP-2.27Q, Planning for Science Activities, and was determined to be quality-affecting and subject to Quality Assurance Requirements and Description (DOE 2004 [DIRS 168669]). These activities are subject to the QARD because they are associated with the characterization of the waste form in support of performance assessment (BSC 2004 [DIRS 167796], Section 8). No special safety management controls, beyond the applicable procedures, apply to this work. The process control evaluations are performed in accordance with AP-SV.1Q, Control of the Electronic Management of Information. The controls on the electronic management of data are implemented in the governing procedures per Section 8 of Technical Work Plan for Waste Form Degradation Modeling, Testing, and Analyses in Support of LA (BSC 2004 [DIRS 167796]). This waste-form FEPs analysis report was developed in accordance with the Office of Repository Development quality assurance program using approved procedures identified in Technical Work Plan for Waste Form Degradation Modeling, Testing, and Analysis in Support of LA (BSC 2004 [DIRS 167796]) and Work Package AWFM01, WF Modeling and Analysis for LA. Additional guidance has been provided in the Scientific Processes Guidelines Manual (BSC 2002 [DIRS 160313]).

Based upon the Q-List, the "waste form/engineered barrier" is considered to be not important to safety but important to waste isolation, and thus has Safety Category "SC" (BSC 2003 [DIRS 165179], Table A-2).

### 3. USE OF SOFTWARE

The analyses and arguments presented herein are based on regulatory requirements, results of analyses presented, and documentation in other scientific analysis reports, model reports, or technical literature and, thus, required no computational software. This report was developed using only commercially available software, used solely for visual display or graphical representation of data, and considered to be controlled under the Software Configuration Control system (LP-SI.11Q-BSC). SigmaPlot, Scientific Graphic Software, Version 3.06, Jandel Corporation, and Microsoft Excel 97 SR-2 are commercial software packages used in this analysis to display the data visually using only standard built-in mathematical functions. SigmaPlot is also used to plot data from the analysis. No calculations are performed with these software packages. No routines or macros were developed using this commercial software. The values used and displayed are approximate and are used only to identify a range of expected values. The analyses in this report provide the basis for the decision to either include or exclude the FEP. If a FEP is to be included in a model, any values or data are developed according to appropriate quality assurance procedures in the applicable subject summary or model abstraction report.

### 4. INPUTS

Section 4.1 and Table 4-1 identify all input data, parameters, and product output used in this analysis. Data and product output have been obtained from controlled source documents and other appropriate sources in accordance with the controlling procedures AP-SIII.9Q and AP-3.15Q. Section 4.2 addresses the FEPs screening criteria and relevant definitions detailed in 10 CFR Part 63 [DIRS 156605] as identified in *Project Requirements Document* (Canori and Leitner 2003 [DIRS 166275]).

### 4.1 DIRECT INPUTS

The information supporting the screening of those LA FEPs dispositioned as "Included" is extracted from WF and WF colloid analysis/model reports identified in this FEPs report and summarized in Table 1.2-1. These reports are direct inputs that explicitly address the disposition of the included FEPs in the TSPA-LA. When cited in this report to support screening decisions to "Exclude" FEPs, the analysis or model reports and other inputs may be used as direct inputs or in a supportive or corroborative manner. Table 4-1 summarized the direct inputs (and Table 6-1 summarizes the indirect inputs) for both included and excluded FEPs. Attachment V contains the qualification of references (per AP-SIII.2Q and AP-SIII.9Q) in Table 4-1 that are not qualified for general use, but are qualified for direct input for use in this analysis report. The LA FEPs often use information developed in those reports as the basis for screening decisions, screening arguments, and TSPA dispositions. Uncertainties in the cited data are considered in the screening of the FEPs in the TSPA-LA. Uncertainties concerning included FEPs are developed in the associated reports.

Table 4-1. Direct Inputs to Waste-Form FEPs Screening Decision to Include

Input	Source	Input Category	Direct Use In	Description
BSC (Bechtel SAIC Company) 2002. Gamma and Neutron Radiolysis in the 21-PWR Waste Package from Ten to One Million Years. 000-00C-DSU0-00700-000A. Las Vegas, Nevada: Bechtel SAIC Company. ACC: MOL.20021004.0002 [DIRS 161912]	entire	Data	Section 6.2.38	Justification in screening out radiolysis due to gamma linear energy transfer (LET) Recent calculations by Tang have shown that neutron irradiation is negligible and gamma dose has been significantly reduced.
BSC (Bechtel SAIC Company) 2002. Radionuclide Screening. ANL-WIS-MD-000006 REV 01. Las Vegas, Nevada: Bechtel SAIC Company. ACC: MOL. 20020923.0017 [DIRS 160059]	entire	Data	Sections 6.2.2, and 6.2.41	The radionuclides of importance to dose calculations were assessed. The assessment considered nominal, human intrusion and igneous events, as well as groundwater and atmospheric exposure scenarios and times.
BSC (Bechtel SAIC Company) 2003. <i>Risk Information to Support Prioritization of Performance Assessment Models</i> . TDR-WIS-PA-000009 REV 01 ICN 01, with errata. Las Vegas, Nevada: Bechtel SAIC Company. ACC: DOC.20031014.0003; MOL.20021017.0045. [DIRS 168796]	Sections 3.3.6 and 3.5.	Data	Section 6.2.3	TSPA parameters and model components that affect dose. Dose is insensitive to DSNF and HLW degradation rates, resulting in low risk prioritization for these components.
BSC (Bechtel SAIC Company) 2003. Dissolved Concentration Limits of Radioactive Elements. ANL-WIS-MD-000010 REV 02. Las Vegas, Nevada: Bechtel SAIC Company. ACC: DOC.20030624.0003 [DIRS 163152]	Section 6.5.1.2	Data	Section 6.2.1	Because waste forms are conservatively considered chemically unchanged, the dissolved concentration of radioelements in water in the basalt would have the same dependency on water chemistry as does waste dissolving in regions not influenced by an igneous intrusion.
	Sections 6.5 through 6.18	Data	Sections 5.2.22 and 6.2.22	Abstracted solubility models for 14 elements (plutonium, neptunium, uranium, thorium, americium, actinium, protactinium, radium, technetium, iodine, strontium, carbon, lead, and cesium) may be used to constrain the maximum radionuclide concentrations.
	entire	Data	Section 6.2.25	Analyses of the relative release rates of neptunium and uranium in the fuel degradation experiments in support of a close correlation between neptunium and uranium concentrations in the leachates
	Section 6.6.4.5	Data	Section 6.2.25	Alternative model (not utilized in the base-case) of incorporation of neptunium into uranyl minerals captures the experimental results very well, and eliminates the built-in conservatism in the conventional pure phase solubility approach and thus gives more realistic source terms.

Table 4-1. Direct Inputs to Waste-Form FEPs Screening Decision to Include (Continued)

Input	Source	Input Category	Direct Use In	Description
	Section 6	Data	Section 6.2.36	Parameterizes dissolved concentrations of radionuclides as a function of in-package and EBS solution chemistry over a range of carbon dioxide partial pressures of $10^{-5}$ to $10^{-1.5}$ — in effect to two orders of magnitude greater than atmospheric.
BSC 2003. DSNF and Other Waste Form Degradation Abstraction. ANL-WIS-MD-000004 REV 02. Las Vegas, Nevada: Bechtel SAIC Company. ACC: DOC.20030711.0002 [DIRS 163693]	entire	Data	Section 6.2.3	DSNF degradation model development.
	Sections 6.4 and 8	Data	Attachment I	N-Reactor SNF represents the overwhelming majority of the DSNF (85%) but less than ~5 % of the total waste to be stored at Yucca Mountain
	Section 6.3	Data	Section 6.2.17	Degradation rates for N-Reactor SNF are adopted as a surrogate for all DSNF. Even when upper bound assumptions for the rate of degradation are used for the entire inventory of DSNF, the contribution of the DSNF to the postclosure site dose, due to degradation and or pyrophoric behavior is negligible.
	Section 6.3	Data	Sections 6.2.6 and 6.2.9	Development of upper-limit, conservative, and best estimate degradation models for each of 11 DSNF waste groups for TSPA-LA.
	Sections 6.3, 6.3.12	Data	Section 6.2.6	Description of immobilized ceramic plutonium waste form.
	Table 9	Data	Section 6.2.19	Rapid corrosion rate of the metallic uranium that is the matrix of N-Reactor SSNF compared with other SNF.
	Section 6.3	Data	Section 6.2.4	The DSNF release rate model has no explicit dependence on water chemistry effects that could result from chemical interactions between or within waste packages.
	Section 7	Data	Section 6.2.6	DSNF degradation model abstraction validation
BSC (Bechtel SAIC Company) 2003. EBS Radionuclide Transport Abstraction. ANL-WIS-PA- 000001 REV 01. Las Vegas, Nevada: Bechtel SAIC Company. [DIRS 162728]	Table 20 and Section 7.5.1	Data	Sections 6.2.34 and 6.2.35	Consideration of dryout near the waste packages, as well as evaporation/condensation within the drift and underneath the drip shield.

21

Table 4-1. Direct Inputs to Waste-Form FEPs Screening Decision to Include (Continued)

Input	Source	Input Category	Direct Use In	Description
BSC (Bechtel SAIC Company) 2004. <i>Igneous Intrusion Impacts on Waste Packages and Waste Forms</i> . MDL-EBS-GS-000002 REV 01D. Las Vegas, Nevada: Bechtel SAIC Company. ACC: MOL.20040414.0095. TBV-5788	Section 6.5.1.1	Data	Section 6.2.1	Igneous intrusion would render the drip shields, waste packages and cladding in the Zone 1 emplacement drifts ineffective so they would provide no further protection to the waste. These evaluations provide further corroboration to the TSPA assumption that the waste packages in Zone 1 provide no further protection to waste forms after an intrusive event.
BSC (Bechtel SAIC Company) 2003. <i>In-Package Chemistry Abstraction</i> . ANL-EBS-MD-000037 REV 02. Las Vegas, Nevada: Bechtel SAIC Company. ACC: DOC.20030723.0003 [DIRS 161962]	entire	Data	Sections 6.2.14, 6.2.15, 6.2.20, 6.2.23, 6.2.24, 6.2.38, and 6.2.40	General reference describing the basis of the conceptual model for in-package chemistry of water.
	Section 6.6.2	Data	Section 6.2.4	Support for the conclusion that DHLWG tends to generate high pH solutions while DOE SNF generates neutral pH solutions, and together combined with the waste package materials the high pH values are buffered to lower values. Also, the DSNF codisposal and high-level radioactive waste glass waste packages are expected to be generally cooler than commercial SNF packages at the time of disposal.
	Table 10 and Sections 6.3.2, 6.3.3, 6.6.1.1, 6.6.1.2, and 6.6.2.2	Data	Section 6.2.21	Support for the conclusion that corrosion products produced during degradation of the waste form metallic portions of the waste package, and metals in the drift (rock bolts, steel in invert, gantry rails) may affect the mobilization and transport of radionuclides.)
	Sections 8.5 and 8.11	Data	Sections 6.2.15 and 6.2.36	Support for the conclusion that it is reasonable to expect little impact of carbon dioxide production on in-package pH and ionic strength, and that only minor amounts of organic matetrials might appear in the WP.
	Sections 4.4.4, 8.2, 8.4, 8.5, and 8.6	Data	Section 6.2.34	Thermodynamic data for EQ6 runs in support of FEP 2.1.11.08.0A.

Table 4-1. Direct Inputs to Waste-Form FEPs Screening Decision to Include (Continued)

Input	Source	Input Category	Direct Use In	Description
BSC (Bechtel SAIC Company) 2003. <i>Initial</i> Radionuclide Inventories. ANL-WIS-MD-000020 REV 00. Las Vegas, Nevada: Bechtel SAIC Company. [DIRS 161961]	Section 6.6 and Table 16	Data	Sections 5.1, 6.2.2, 6.2.3, 6.2.5, 6.2.18 and 6.2.41	Provides the inventories of radionuclides for three major categories of waste forms, currently planned for disposal at Yucca Mountain: CSNF, DSNF, and DHLW Glass.
BSC (Bechtel SAIC Company) 2003. Waste Form and In-Drift Colloids-Associated Radionuclide Concentrations: Abstraction and Summary. MDL-EBS-PA-000004 REV 00 ICN 01. Las Vegas, Nevada: Bechtel SAIC Company. ACC: DOC.20031222.0012 [DIRS 166845]	Sections 5.9, 6.3.1, 6.3.2, 6.3.3, and 6.3.4	Data	Sections 5.2.30, 6.2.21, 6.2.27, 6.2.28, 6.2.29, 6.2.30, 6.2.31, and 6.2.32	Effect of waste form colloids-associated concentrations on chemical interactions.
BSC (Bechtel SAIC Company) 2004. FEPs Screening of Processes and Issues in Drip Shield and Waste Package Degradation. ANL-EBS-PA-000002 REV 02. Las Vegas, Nevada: Bechtel SAIC Company. ACC: DOC.20040408.0001. [DIRS 162200]	Section 6.2.13.5	Data	Section 6.2.37	Maximum allowable waste package interior pressures due to the release of radioactive gases to the interior of the waste package will be too low to damage the waste package.
BSC (Bechtel SAIC Company) 2004. CSNF Waste Form Degradation: Summary Abstraction. ANL-EBS-MD-000015 REV 01, with errata. Las Vegas, Nevada: Bechtel SAIC Company. ACC: DOC.20030708.0004; DOC.20031224.0001; DOC.20040202.0002 [DIRS 167321]	Sections 1, 6.2, 6.2.2.3, 6.4.1.5	Data	Sections 6.2.6 6.2.7, and 6.2.12	Characteristics of CSNF waste degradation processes and CSNF degradation model.
BSC (Bechtel SAIC Company) 2004. <i>Multiscale Thermohydrologic Model.</i> ANL-EBS-MD-000049 REV 01. Las Vegas, Nevada: Bechtel SAIC Company. ACC: DOC.20040301.0004. [DIRS 163056]	entire	Data	Section 6.2.34	Thermal effects on liquid or two-phase flow within the waste and EBS are explicitly accounted for in the Multiscale Thermohydrologic Model. Explicit accounting for thermal effects on liquid or two-phase flow within the waste and EBS, including consideration of dryout near the waste packages, as well as evaporation/condensation within the drift and underneath the drip shield.
BSC (Bechtel SAIC Company) 2004. Defense HLW Glass Degradation Model. ANL-EBS-MD-000016 REV 01 ICN 01. Las Vegas, Nevada: Bechtel SAIC Company. ACC: DOC.20040223.0006 [DIRS 167619]	Sections 6.5.2 and 6.5.4.2	Data	Section 6.2.3 and 6.2.5	The effect of waste glass compositions on the calculated degradation rate is taken into account through the range of values of the model parameter KE. Ranges for the values of KE in acidic and alkaline solutions are selected based on the results of laboratory tests with glasses that provide a wide range of compositions that bounds the range of concentrations of key glass components in DHLW glasses, such as aluminum. The glass degradation model accounts for the heterogeneity of the waste

Table 4-1. Direct Inputs to Waste-Form FEPs Screening Decision to Include (Continued)

Input	Source	Input Category	Direct Use In	Description
				inventory.
	Section 8.2.2	Data	Section 6.2.3 and 6.2.8	The glass degradation model addresses degradation of glass exposed to humid air and dripping water, and glass immersed in water. The glass degradation rate is calculated as a function of pH and temperature.
	Section 8.2.1	Data	Sections 6.2.4 and 6.2.10	The surface area used to calculate the radionuclide release rate bounds the effects of thermal cracking during manufacture and impact cracking during subsequent handling. The exposure factor (fexposure) is used to model the combined effects of the added surface area due to cracking, the fraction of the surface that is accessible to water, and the reactivity of glass in tight cracks relative to glass at a free surface.
	Section 7.5.1 and Table 7.5-1	Data	Section 6.2.11	The glass degradation model is insensitive to the presence of crystalline phases that are either formed by devitrification of the glass melt during manufacture or intentionally added to the waste form.
	Sections 6.5.4.1 and 6.5.4.3	Data	Section 6.2.21	The effects of dissolved iron on the glass dissolution rates are addressed by using the results of tests in which iron products were added to the test solution when determining model parameter values for pH dependence $(f\Omega)$ in acidic and alkaline solutions. The effects of glass alteration phases on the glass dissolution rate are addressed by including the results of tests in which alteration phases form when determining model parameter values for KE.
	Section 7.5	Data	Section 6.2.1	HLW glass degradsation rate in water would not be significantly affected by the types of crystalline inclusion phases that could form during the slow cooling of the HLW glass exposed to Zone 2 conditions.
CRWMS M&O 1999. BWR Source Term Generation and Evaluation. BBAC00000-01717-0210-00006 REV 01. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.200000113.0334 [DIRS 136428]	Attachment XV	Data	Attachment IV	BWR radionuclide source term.

Table 4-1. Direct Inputs to Waste-Form FEPs Screening Decision to Include (Continued)

Input	Source	Input Category	Direct Use In	Description
CRWMS M&O 1999. PWR Source Term Generation and Evaluation. BBAC00000-01717-0210-00010 REV 01. Las Vegas, Nevada: CRWMS M&O. acc: MOL.20000113.0333 [DIRS 136429]	Attachment XV	Data	Attachment IV	PWR radionuclide source term.
CRWMS M&O 2000. <i>In-Drift Microbial Communities</i> . ANL-EBS-MD-000038 REV 00 ICN 01. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.20001213.0066 [DIRS 151561]	Sections 6.3 and 7	Data	Sections 6.2.26 and 6.2.34	Estimates of microbe massses growing in the repository system suggest that the effects on the bulk in-drift geochemistry should be small. Bounding biomass estimates are ~100grams (dry) per meter of drift; insufficient to produce high chelate levels.
DOE (U.S. Department of Energy) 2002. DOE Spent Nuclear Fuel Information in Support of TSPA-SR. DOE/SNF/REP-047, Rev. 2. Idaho Falls, Idaho: U.S. Department of Energy, Idaho Operations Office. ACC: DOC.20030905.0020 [DIRS 158405]	Section 6.2	Data	Attachment I	Uranium-metal spent fuel more chemically reactive than other spent fuel.
	Appendix D	Data	Section 6.2.6, 6.2.17, and 6.2.18	The total inventory of the Group 3 (Pu/U carbide) SNF is less than .001 % of DSNF waste.
	Section 9	Data	Section 6.2.3 and 6.2.4	Current plans call for five glass logs and one DSNF canister to be placed in each codisposal package.
DOE (U.S. Department of Energy) 2002. <i>Yucca Mountain Science and Engineering Report.</i> DOE/RW-0539, Rev. 1. Washington, D.C.: U.S. Department of Energy, Office of Civilian Radioactive Waste Management. ACC: MOL.20020404.0042.	Section 1.4.2.2.2	Established Fact	Section 6.2.18	Description of repository site bedrock geology.
Rechard, R.P., ed. 1995. Methodology and Results. Volume 2 of Performance Assessment of the Direct Disposal in Unsaturated Tuff of Spent Nuclear Fuel and High-Level Waste Owned by U.S. Department of Energy. SAND94-2563/2. Albuquerque, New Mexico: Sandia National Laboratories. TIC: 237102 [DIRS 101084]	Section 11.3.1, pp. 11 to 24	Data (qualified per Attachment V)	Sections 6.2.6 and 6.2.16	Significant amounts of DSNF cladding are likely to be damaged
Sunder, S.; Shoesmith, D.W.; and Miller, N.H. 1997. "Oxidation and Dissolution of Nuclear Fuel (UO <sub>2</sub> ) by the Products of the Alpha Radiolysis of Water." <i>Journal of Nuclear Materials</i> , 244, 66-74. Amsterdam, The Netherlands: Elsevier. TIC: 246914. [DIRS 143860]	pp. 67 to 74	Data (qualified per Attachment V)	Section 6.2.38	Support for the conclusion that the effects of alpha radiolysis on spent fuel corrosion (dissolution) will be transitory and will become minor as alpha dose rates decrease

Table 4-1. Direct Inputs to Waste-Form FEPs Screening Decision to Include (Continued)

Input	Source	Input Category Direct Use In	Direct Use In	Description
Thornton, T.A. 1998. "HPPP Issue 1; Preliminary TSPA for a Pyrophoric Event Involving N-Reactor SNF Waste Packages." Interoffice correspondence from T.A. Thornton (CRWMS M&O) to J.S. Clouet, S.S. Sareen, and D. Stahl, September 21, 1998, LV.WP.TAT.09/98-179, with attachment. MOL. 19981019.0001 [DIRS 125082]	entire	Data (qualified per Attachment V)	Section 6.2.13	Data (qualified Section 6.2.13 Examples of the potential for pyrophoric behavior in uranium metal and uranium metal-based spent nuclear fuel.
DTN: MO0402SPAHWCIG.002. Heat and Water Chemistry Output From Igneous Intrusion. Submittal date: 02/23/2004. [DIRS 168762]	entire	Data	Section 6.2.1	Temperatures of waste forms as they are disributed through the magma as the result of an igneous event.

#### 4.2 CRITERIA

The NRC provides guidance in *Yucca Mountain Review Plan, Final Report* (NRC 2003 [DIRS 163274]) in accordance with 10 CFR 63.114(d), (e), and (f) [DIRS 156605] on the screening process to exclude FEPs. The guidance states criteria that will be used as follows (Section 2.2.1.2.1.3):

**Acceptance Criterion 1**—The Identification of a List of Features, Events, and Processes Is Adequate

• The Safety Analysis Report contains a complete list of features, events, and processes, related to the geologic setting or the degradation, deterioration, or alteration of engineered barriers (including those processes that would affect the performance of natural barriers), that have the potential to influence repository performance. The list is consistent with the site characterization data. Moreover, the comprehensive features, events, and processes list includes, but is not limited to, potentially disruptive events related to igneous activity (extrusive and intrusive); seismic shaking (high-frequency-low magnitude, and rare large-magnitude events); tectonic evolution (slip on existing faults and formation of new faults); climatic change (change to pluvial conditions); and criticality.

#### **How Addressed**

FEPs related to the WF and WF colloid processes evaluated in this report are listed in Table 1.2-1. Those subject matter analysis model reports that provide supporting technical discussions relevant to a specific FEP are identified in the table. Documentation of the evolution of the YMP FEP list is provided in Section 1.2.1.

**Acceptance Criterion 2**—Screening of the List of Features, Events, and Processes Is Appropriate

- The U.S. Department of Energy has identified all features, events, and processes related to either the geologic setting or to the degradation, deterioration, or alteration of engineered barriers (including those processes that would affect the performance of natural barriers) that have been excluded;
- The U.S. Department of Energy has provided justification for those features, events, and processes that have been excluded. An acceptable justification for excluding features, events, and processes is that either the feature, event, and process is specifically excluded by regulation; probability of the feature, event, and process (generally an event) falls below the regulatory criterion; or omission of the feature, event, and process does not significantly change the magnitude and time of the resulting radiological exposures to the reasonably maximally exposed individual, or radionuclide releases to the accessible environment; and
- The U.S. Department of Energy has provided an adequate technical basis for each feature, event, and process, excluded from the performance assessment, to support the

conclusion that either the feature, event, or process is specifically excluded by regulation; the probability of the feature, event, and process falls below the regulatory criterion; or omission of the feature, event, and process does not significantly change the magnitude and time of the resulting radiological exposures to the reasonably maximally exposed individual, or radionuclide releases to the accessible environment.

#### **How Addressed**

The above criterion permits an exclusion argument for FEPs that are not consistent with the regulations because of waste characteristics, repository design, or site characteristics, provided NRC staff finds sufficient justification. Additionally, a FEP may be excluded from TSPA-LA if it is demonstrated that the likelihood of a specific occurrence is below the quantitative probability of one in 10,000 of occurring over a period of 10,000 years. The final criterion permits exclusion of FEPs that do not significantly change the calculated expected annual dose provided the NRC staff finds sufficient support in accompanying discussions or calculations, including the use of either bounding or representative estimates. The sequence implemented in excluding a WF FEP is provided in Section 6.1. Generally, a regulatory-type screening criterion was examined first, followed by a screening rationale based on either a low probability or a low consequence criterion. In Section 6.2 are brief discussions, labeled as "Screening Arguments," providing the rationale for excluding a FEP. A summary of screening arguments and the exclusion basis is provided in Section 6.

#### 4.2.1 Regulatory Basis for NRC Guidance

This scientific analysis report complies with the NRC's criteria for FEP screening, given in 10 CFR Part 63 [DIRS 156605]. The criteria that can be used to exclude a FEP from TSPA-LA are given in the following subsections.

## 4.2.1.1 Low Probability Criterion

The low probability criterion is explicitly stated in 10 CFR 63.114(d) [DIRS 156605]:

Consider only events that have at least one chance in 10,000 of occurring over 10,000 years.

and supported by 10 CFR 63.342 [DIRS 156605]:

DOE's performance assessments shall not include consideration of very unlikely features, events, or processes, i.e., those that are estimated to have less than one chance in 10,000 of occurring within 10,000 years of disposal.

The low-probability criterion (i.e., very unlikely FEPs) is stated as less than one chance in 10,000 of occurring in 10,000 years (i.e.,  $10^{-4}/10^4$  yr, or a probability of  $10^{-8}$ ).

Furthermore, it is stated in 10 CFR 63.342 [DIRS 156605] that:

DOE's assessments for the human-intrusion and ground-water protection standards shall not include consideration of unlikely features, events, or processes, or sequences of events and processes, i.e., those that are estimated to have less than one chance in 10 and at least one chance in 10,000 of occurring within 10,000 years of disposal.

This criterion for unlikely FEPs corresponds to an annualized probability of less than  $10^{-5}$ , but greater than or equal to  $10^{-8}$ , which is the upper boundary for very unlikely FEPs.

## 4.2.1.2 Low-Consequence Criteria

Criteria for low-consequence screening arguments are provided in 10 CFR 63.114(e) and (f) [DIRS 156605], which indicates that performance assessments shall:

- (e) Provide the technical basis for either inclusion or exclusion of specific features, events, and processes in the performance assessment. Specific features, events, and processes must be evaluated in detail if the magnitude and time of the resulting expected radiological exposures to the reasonably maximally exposed individual, or radionuclide releases to the accessible environment, would be significantly changed by their omission.
- (f) Provide the technical basis for either inclusion or exclusion of degradation, deterioration, or alteration processes of engineered barriers in the performance assessment, including those processes that would adversely affect the performance of natural barriers. Degradation, deterioration, or alteration processes of engineered barriers must be evaluated in detail if the magnitude and time of the resulting radiological exposures to the reasonably maximally exposed individual, or radionuclide releases to the accessible environment, would be significantly changed by their omission.

Furthermore, it is stated in 10 CFR 63.342 [DIRS 156605] that

DOE's performance assessments need not evaluate the impacts resulting from any features, events, and processes or sequences of events and processes with a higher chance of occurrence if the results of the performance assessments would not be changed significantly.

Because the relevant performance measures differ for different FEPs (e.g., effects on performance can be measured in terms of changes in concentrations, flow rates, transport times, or other measures as well as overall expected annual dose), there is no single quantitative test of "significance."

Some FEPs have a beneficial effect on the TSPA, as opposed to an adverse effect. As identified in 10 CFR 63.102(j) [DIRS 156605], the concept of a performance assessment includes that:

The features, events, and processes considered in the performance assessment should represent a wide range of both beneficial and potentially adverse effects on performance (e.g., beneficial effects of radionuclide sorption; potentially adverse effects of fracture flow or a criticality event). Those features, events, and processes expected to materially affect compliance with [10 CFR] 63.113(b) or be

potentially adverse to performance are included, while events (event classes or scenario classes) that are very unlikely (less than one chance in 10,000 over 10,000 years) can be excluded from the analysis. ...

Yucca Mountain Review Plan, Final Report (NRC 2003 [DIRS 163274], Section 2.2.1), states:

In many regulatory applications, a conservative approach can be used to decrease the need to collect additional information or to justify a simplified modeling approach. Conservative estimates for the dose to the reasonably maximally exposed individual may be used to demonstrate that the proposed repository meets U.S. Nuclear Regulatory Commission regulations and provides adequate protection of public health and safety. ...The total system performance assessment is a complex analysis with many parameters, and the U.S. Department of Energy may use conservative assumptions to simplify its approaches and data collection needs. However, a technical basis...must be provided.

On the basis of these statements, those FEPs that are demonstrated to have only beneficial effects on the radiological exposures to the reasonably maximally exposed individual, or radionuclide releases to the accessible environment, can be excluded on the basis of low consequence because they have no adverse effects on performance.

#### 4.2.1.3 By-Regulation Criteria

Regulations which specify characteristics, concepts, and definitions may serve as the basis for exclusion of FEPs by regulation, as allowed by *Yucca Mountain Review Plan, Final Report* (NRC 2003 [DIRS 163274]). These include the characteristics, concepts and definitions pertaining to the reference biosphere and geologic setting and the RMEI. Also pertinent are characteristics, concepts, and definitions that must be considered during the FEP screening, such as the areal extent of the accessible environment and of the controlled area, and the spatial relationship to the distance from the repository to the RMEI.

#### 4.3 CODES AND STANDARDS

There are no formally established codes or standards directly applicable to this analysis. Regulations used by the DOE to set conformance criteria are in:

• 10 CFR 63. Energy: Disposal of High-Level Radioactive Wastes in a Geologic Repository at Yucca Mountain, Nevada. [DIRS 156605]

#### 5. ASSUMPTIONS

#### 5.1 GENERAL ASSUMPTIONS

There are two general assumptions used indirectly throughout this analysis model report in screening WF FEPs. These assumptions are not specific to the disposition of any single FEP but rather are used throughout the FEP analyses contained in Section 6.2 of this report. These general assumptions do not need further confirmation.

## 5.1.1 Consistency with Design

Assumption: The TSPA is based on an assumption that the repository will be constructed, operated, and closed according to the design used as the basis for the FEP screening.

Rationale: Unless a FEP can be excluded because of a low probability of the phenomenon ever occurring, the FEP screening decision is based, at least in part, on the waste package design in Waste Package Design Methodology Report (McKenzie 2002 [DIRS 158010]). This assumption is justified because a only a major change in the waste package or EBS design would require a reevaluation of the screening decision for FEPs dependent on design requirements.

Confirmation Status: Confirmation is not required for this general assumption.

*Use in the Analysis*: This general assumption is used throughout the report.

## **5.1.2** Waste Type and Inventory

Assumption: Only the wastes described in *Initial Radionuclide Inventories* (BSC 2003 [DIRS 161961]) were considered in these analyses.

*Rationale*: This assumption is based on the fact that *Initial Radionuclide Inventories* (BSC 2003 [DIRS 161961]) represents the latest compilation of waste forms.

Confirmation Status: Confirmation is not required for this general assumption.

Use in the Analysis: This general assumption is used throughout the report.

#### 5.2 FEPS-SPECIFIC ASSUMPTIONS

## 5.2.1 Igneous Intrusion Interacts with EBS Components (1.2.04.04.0A)

It is conservatively assumed in addressing this FEP that the igneous intrusion would render the drip shields, waste packages, cladding, and waste forms in Zone 1 emplacement drifts ineffective as barriers, providing no further protection to the waste and that contact with magma causes the waste form to be distributed throughout the cooled magma leaving the waste forms chemically unchanged, and thus that the dissolved concentration of radioelements in water has the same dependency on water chemistry as for waste not contacted by magma. This assumption is used in Section 6.2.1 to support the screening decision to include this FEP. The assumption, since it is conservative with respect to the calculation of dose, does not require confirmation.

#### **5.2.2** Waste Inventory (2.1.01.01.0A)

No assumptions were used in addressing this FEP.

## 5.2.3 Interactions between Colocated Waste (2.1.01.02.0A)

No assumptions were used in addressing this FEP.

### 5.2.4 Interactions Between Codisposed Waste (2.1.01.02.0B)

No assumptions were used in addressing this FEP.

#### 5.2.5 Heterogeneity of Waste Inventory (2.1.01.03.0A)

No assumptions were used in addressing this FEP.

# 5.2.6 DSNF Degradation (Alteration, Dissolution, and Radionuclide Release) (2.1.02.01.0A)

It is conservatively assumed in addressing this FEP that the cladding of the DSNF provides no retardation of the degradation of the SNF upon contact with water. This assumption is primarily based on observations of the extent of cladding damage to N-Reactor SNF. This assumption is used in Section 6.2.6 to support the screening decision to include this FEP in the TSPA-LA. The assumption requires no further confirmation because it represents the worst possible cladding condition for the DSNF.

# 5.2.7 CSNF Degradation (Alteration, Dissolution, and Radionuclide Release) (2.1.02.02.0A)

No assumptions were used in addressing this FEP.

# 5.2.8 HLW Glass Degradation (Alteration, Dissolution, and Radionuclide Release) (2.1.02.03.0A)

No assumptions were used in addressing this FEP.

### 5.2.9 Alpha Recoil Enhances Dissolution (2.1.02.04.0A)

No assumptions were used in addressing this FEP.

#### 5.2.10 HLW Glass Cracking (2.1.02.05.0A)

No assumptions were used in addressing this FEP.

### 5.2.11 HLW Glass Recrystallization (2.1.02.06.0A)

No assumptions were used in addressing this FEP.

## 5.2.12 Radionuclide Release From Gap and Grain Boundaries (2.1.02.07.0A)

No assumptions were used in addressing this FEP.

## **5.2.13** Pyrophoricity from DSNF (2.1.02.08.0A)

Any actual breach of the waste package and container holding the potentially pyrophoric N-Reactor SNF would probably be small enough such that exposure of the SNF to air or water vapor would occur slowly and thereby limit the rate of reaction, since the waste package and container are initially sealed with an inert gas. However, for the purpose of estimating the potential effect of pyrophoricity on release, it is conservatively (but non-mechanistically) assumed that all N-Reactor SNF-containing waste packages that breach during the regulatory period undergo a pyrophoric event within one TSPA time step. It is also assumed that (1) breach of an N-Reactor SNF-containing waste package results in a pyrophoric condition that causes the two adjacent waste packages to fail, (2) the various types of waste packages are evenly distributed throughout the repository, and (3) the probability of failure of a waste package containing pyrophoric (i.e., N-Reactor) SNF is the same as that of any other waste package. This assumption is used in Section 6.2.13 and Attachment I to provide partial support to the screening argument decision to exclude this FEP from the TSPA-LA. This assumption requires no confirmation because it conservatively represents the worst possible effect of the pyrophoric event on adjacent waste packages.

## 5.2.14 Chemical Effects of Void Space in the Waste Package (2.1.02.09.0A)

No assumptions were used in addressing this FEP.

#### 5.2.15 Organic/Cellulosic Materials in Waste (2.1.02.10.0A)

No assumptions were used in addressing this FEP.

## **5.2.16 DSNF Cladding (2.1.02.25.0A)**

It is assumed in this FEP that the DSNF cladding does not provide a retardation barrier to the release of radionuclides. This is based on the observation of significant amounts of damage to the N-Reactor SNF (over 80 percent by weight of all DSNF) cladding (Abrefah et al. 1995 [DIRS 151125]), and the fact that there has been insufficient characterization of the various other types of DSNF cladding to establish it as intact for the purpose of the TSPA-LA. This assumption is used in Section 6.2.16 to support the designation of this FEP as excluded. This assumption requires no confirmation because it conservatively recommends the worst possible cladding condition for use in the analysis.

# 5.2.17 Grouping of DSNF Waste Types into Categories (2.1.02.28.0A)

In addressing this FEP, it is assumed that the entire DSNF inventory (with the exception of naval SNF) can be conservatively represented by N-Reactor SNF. The basis for this assumption is that the rate of degradation of the N-Reactor SNF can be shown to be higher than all but a miniscule fraction of the rest of the DSNF. This assumption is used in Section 6.2.17 to support the screening decision to include this FEP in the TSPA-LA. This assumption does not require

further confirmation because it represents a bounding condition for use in the analysis of all the DSNF types.

#### 5.2.18 Flammable Gas Generation from DSNF (2.1.02.29.0A)

No assumptions were used in addressing this FEP.

# 5.2.19 Internal Corrosion of Waste Packages Prior to Breach (2.1.03.06.0A)

In addressing this FEP it is assumed that only a limited amount of water will be allowed by waste acceptance criteria inside a waste package. This assumption is based on the planned inert gas backfill of waste packages and containers. This assumption is used in Section 6.2.19 to support the screening decision to exclude this FEP from the TSPA-LA. It does not require confirmation because waste acceptance criteria do not allow for damaged waste packages and limit the amount of water in undamaged waste packages.

## 5.2.20 Chemical Characteristics of Water in Waste Package (2.1.09.01.0B)

No assumptions were used in addressing this FEP.

#### 5.2.21 Chemical Interaction with Corrosion Products (2.1.09.02.0A)

No assumptions were used in addressing this FEP.

# 5.2.22 Radionuclide Solubility, Solubility Limits, and Speciation in the Waste Form and EBS (2.1.09.04.0A)

In addressing this FEP it is conservatively assumed that under repository condition no strontium solubility-controlling solid exists and its release is considered to be controlled by the dissolution rate of waste forms and the waste inventory (BSC 2003 [DIRS 163152], Section 6.18). The basis for this assumption is that strontium is quite soluble and it does not contribute to dose significantly. This assumption is used in Section 6.2.22 to support the screening argument to include this FEP in the TSPA. This assumption is conservative and is supported by *Dissolved Concentration Limits of Radioactive Elements* (BSC 2003 [DIRS 163152]) and so requires no further confirmation for its usage in this document.

## 5.2.23 Reduction-Oxidation Potential in Waste Package (2.1.09.06.0A)

No assumptions were used in addressing this FEP.

## 5.2.24 Reaction Kinetics in Waste Package (2.1.09.07.0A)

No assumptions were used in addressing this FEP.

## 5.2.25 Secondary Phase Effects on Dissolved Radionuclide Concentrations (2.1.09.10.0A)

In addressing this FEP it is assumed that the constant ratio of neptunium to uranium in the leachate is the result of the formation of solid solutions in the secondary uranium phases. The basis for this assumption is the experimental observations that the neptunium and uranium

behave coherently both in the release from the waste form and in the process of secondary phase formation, and this results in lower neptunium concentrations observed in the leachate than would be expected from solubility limits. This assumption is used in Section 6.2.25 to demonstrate that the use of the mechanistic model for the dissolution/precipitation reactions are conservative in terms of predicting neptunium transport, and therefore support the screening argument to exclude this FEP from TSPA. This assumption is supported by *Dissolved Concentration Limits of Radioactive Elements* (BSC 2003 [DIRS 163152]) and so requires no further confirmation for its usage in this document.

## **5.2.26** Complexation in EBS (2.1.09.13.0A)

No assumptions were used in addressing this FEP.

## 5.2.27 Formation of True (Intrinsic) Colloids in EBS (2.1.09.15.0A)

No assumptions were used in addressing this FEP.

## 5.2.28 Formation of Pseudo-Colloids (Natural) in EBS (2.1.09.16.0A)

No assumptions were used in addressing this FEP.

#### 5.2.29 Formation of Pseudo-Colloids (Corrosion Product) in EBS (2.1.09.17.0A)

No assumptions were used in addressing this FEP.

### 5.2.30 Formation of Microbial Colloids in EBS (2.1.09.18.0A)

The potential influence of organic complexants from microbial metabolism on radionuclide transport is assumed not to affect the stability of inorganic (mineral) colloids (BSC 2003 [DIRS 166845], Sections 5.9 and 6.3.4) (i.e., inorganic colloid stability is determined by fluid chemistry [ionic strength and pH]). Therefore this assumption is used in section 6.2.30 to support the decision to exclude this FEP on the basis of low consequence. This assumption is supported by the analyses in *Waste Form and In-Drift Colloids-Associated Radionuclide Concentrations: Abstraction and Summary* (BSC 2003 [DIRS 166845]) and so does not require further confirmation for its usage in this report.

#### **5.2.31** Stability of Colloids in EBS (2.1.09.23.0A)

No assumptions were used in addressing this FEP.

## 5.2.32 Formation of Colloids (Waste-Form) by Coprecipitation in EBS (2.1.09.25.0A)

No assumptions were used in addressing this FEP.

### 5.2.33 Exothermic Reactions in the EBS (2.1.11.03.0A)

No assumptions were used in addressing this FEP.

## 5.2.34 Thermal Effects on Chemistry and Microbial Activity in the EBS (2.1.11.08.0A)

No assumptions were used in addressing this FEP.

## 5.2.35 Thermally Driven Flow (Convection) in the EBS (2.1.11.09.0B)

It is assumed in addressing this FEP that a single mixing cell in the waste package may be used for determining transport out of the waste package. The basis for this assumption is the determination that thermal convection inside the waste package would tend to erase concentration gradients and distribute radionuclides uniformly throughout the package. This assumption is used in Section 6.2.35 to support the screening argument to exclude this FEP from the TSPA-LA. This assumption does not require validation because having the concentration of dissolved materials dispersed uniformly would slightly over-predict the transport of radionuclides out of the waste package, and is thus conservative.

# 5.2.36 Gas Generation (CO<sub>2</sub>, CH<sub>4</sub>, and H<sub>2</sub>S) from Microbial Degradation (2.1.12.04.0A)

In addressing this FEP it is assumed that the potential impacts of high carbon dioxide levels from microbial degradation on radioactive element solubilities will be small. The basis for this assumption is the analysis of dissolved concentrations of radioactive elements by Finch and Fortner (2002 [DIRS 162004]), which encompassed carbon dioxide partial pressures as high as 1.0 to 1.5 atmospheres. This analysis showed this effect to be small. This assumption is used in Section 6.2.36 in support of the screening decision to exclude this FEP from the TSPA-LA based on low consequence.

## 5.2.37 Effects of Radioactive Gases in EBS (2.1.12.07.0A)

No assumptions were used in addressing this FEP.

## **5.2.38** Radiolysis (2.1.13.01.0A)

No assumptions were used in addressing this FEP.

### **5.2.39** Radiation Damage in EBS (2.1.13.02.0A)

No assumptions were used in addressing this FEP.

### 5.2.40 Chemistry of Water Flowing into Waste Package (2.2.08.12.0B)

No assumptions were used in addressing this FEP.

#### 5.2.41 Radioactive Decay and In-Growth (3.1.01.01.0A)

No assumptions were used in addressing this FEP.

#### 6. SCIENTIFIC ANALYSIS DISCUSSION

This analysis model report addresses the 41 FEPs that have been identified as waste-form FEPs. These FEPs generally represent waste form and colloid formation processes that are potentially relevant to repository performance. FEPs representing cladding processes are addressed elsewhere (BSC 2003 [DIRS 165057]).

For FEPs that are excluded based on 10 CFR Part 63 [DIRS 156605], the screening argument identifies the exclusion criterion (low probability [Section 4.2.1.1] or low consequence [Section 4.2.1.2]) and provides a short summary of the technical basis. No waste-form FEPs have an excluded screening decision based solely on regulatory requirements or regulatory-specified conditions (Section 4.2.1.3).

For FEPs that are included in the TSPA, the disposition describes how the FEP has been incorporated in the TSPA model, either directly or through an abstraction. Supporting analysis or model reports that provide a more detailed discussion of the implementation of included FEPs are also identified.

Corroborating and supporting information used in this scientific analysis activity is listed and statused in Table 6-1. This report identifies all sources of corroborating or supporting information used in this model report. No explicit calculations using product output or technical information were performed as a part of this activity, so the analysis of uncertainties is not involved

Table 6-1. Supporting Information for Waste-Form FEPs Disposition

DIRS Number	Accession or TIC number	Reference	Used From	Type of Information	Description
151125	243197	Abrefah, J.; Gray, W.J.; Ketner, G.L.; Marschman, Section 3.1 and S.C.; Pyecha, T.D.; and Thornton, T.A. 1995. <i>K-Basin Spent Nuclear Fuel Characterization Data Report</i> . PNL-10778. Richland, Washington: Pacific Northwest National Laboratory.	Section 3.1 and Figures 3.1 to 3.5	corroborating/ supporting	Evidence that a significant fraction of the N-Reactor spent fuel is currently damaged and so will be damaged at the time of emplacement in the repository.
151226	248558	Abrefah, J.; Huang, F.H.; Gerry, W.M.; Gray, W.J.; Marschman, S.C.; and Thornton, T.A. 1999. <i>Analysis of Ignition Testing on K-West Basin Fuel.</i> PNNL-11816. Richland, Washington: Pacific Northwest National Laboratory.	entire	supporting/	There is a small but finite chance of spontaneous ignition of N-Reactor SNF since uranium hydride inclusions tend to be concentrated near the exposed uranium metal fuel surface of damaged U-metal SNF. Because the fraction of N-Reactor SNF with cladding damaged enough to expose the metallic uranium core is quantitatively unknown but potentially significant, essentially all the SNF elements can be regarded as damaged for the purposes of this analysis.
			Tables 4.2, 4.3	corroborating/ supporting	The presence of uranium hydride inclusions are believed to be responsible for the observed decreased ignition temperature observed during ignition testing of damaged/corroded N-Reactor SNF samples compared to unirradiated/undamaged samples.
163864	MOL.20030 619.0100	Adkins, H.E. 2003. "Transmittal of Draft Version of Validation of Dissolved Concentrations, Argonne National Laboratory." Interoffice memorandum from H.E. Adkins (BSC) to Y. Chen, June 19, 2003, 0617037708, with attachment.	entire	corroborating/ supporting	Draft Input - Validation of Dissolved Concentrations, Argonne National Laboratory.
152779	248977	ASTM C 1454-00. 2000. Standard Guide for Pyrophoricity/Combustibility Testing in Support of Pyrophoricity Analyses of Metallic Uranium Spent Nuclear Fuel. West Conshohocken, Pennsylvania: American Society for Testing and Materials.	entire	corroborating/ supporting	ASTM Standard Guide for evaluating the potential for pyrophoric behavior of uranium metal-based spent fuel.

Table 6-1. Supporting Information for Waste-Form FEPs Disposition (Continued)

DIRS Number	Accession or TIC number	Reference	Used From	Type of Information	Description
101565	240716	Bruno, J.; Cera, E.; Eklund, UB.; Eriksen, T.E.; and Grive, M. 1998. Some Preliminary Modeling Results of Long Term Radiolytic Mass Balance Experiments. Presentation at the Spent Fuel Workshop 1998, Las Vegas, Nevada, May 18-20, 1998. [Barcelona, Spain]: Quantisci.	entire	corroborating/ supporting	Observation that a coherent relationship exists between neptunium and uranium in spent fuel dissolution experiments in the Spanish Nuclear Waste Program in support of the conclusion that the ratio of neptunium to uranium in the leachate is equal to the ratio in the spent fuel used in experiments.
162733	MOL.20020 107.0156	BSC (Bechtel SAIC Company) 2001. In-Drift Microbial Communities Model Validation Calculations. CAL-EBS-EV-000001 REV 00 ICN 02. Las Vegas, Nevada: Bechtel SAIC Company.	entire	corroborating/ supporting	Calculated microbial populations will not be sufficient to generate significant concentrations of radionuclide-chelating organics
153755	MOL.20010 629.0076	BSC (Bechtel SAIC Company) 2001. Internal Pressurization Due to Fuel Rod Rupture in Waste Packages. CAL-EBS-ME-000005 REV 01. Las Vegas, Nevada: Bechtel SAIC Company.	Section 6, Table 6- 1	corroborating/ supporting	Support for the conclusion that partial pressures from radioactive gas will not be great enough to compromise waste package integrity that would result in a waste package breach.
168795	DOC.20031 014.0005	BSC (Bechtel SAIC Company) 2003. <i>In-Package Chemistry for Waste Forms</i> . ANL-EBS-MD-000056 REV 00, with errata. Las Vegas, Nevada: Bechtel SAIC Company.	Attachment II	corroborating/ supporting	Supports screening out gamma radiation as affecting radiation changes in waste
165057	DOC.20040 322.0001	BSC (Bechtel SAIC Company) 2003. <i>Clad Degradation – FEPs Screening Arguments</i> . ANL-WIS-MD-000008 REV 01. Las Vegas, Nevada: Bechtel SAIC Company.	entire	corroborating/ supporting	Cladding FEPs screening arguments
			Appendix A, Table A-3	corroborating/ supporting	WP temperature grasdients will be low at 1000 years.
167619	DOC.20040 223.0006	BSC (Bechtel SAIC Company) 2004. Defense HLW Glass Degradation Model. ANL-EBS-MD-000016 REV 01 ICN 01. Las Vegas, Nevada: Bechtel SAIC Company.	entire	corroborating/ supporting	Summary table indicating FEPs which Model Report helps resolve.
163152	DOC.20030 624.0003	BSC (Bechtel SAIC Company) 2003. Dissolved Concentration Limits of Radioactive Elements. ANL-WIS-MD-000010 REV 02. Las Vegas, Nevada: Bechtel SAIC Company.	Section 6.2, Table 6.2-1	corroborating/ supporting	Description of solubility FEP
163693	DOC.20030 711.0002	BSC (Bechtel SAIC Company) 2003. DSNF and Other Waste Form Degradation Abstraction.	entire	corroborating/ supporting	WF FEPs-related model reports

Table 6-1. Supporting Information for Waste-Form FEPs Disposition (Continued)

DIRS	Accession or TIC number	Reference	Used From	Type of Information	Description
		ANL-WIS-MD-000004 REV 02. Las Vegas, Nevada: Bechtel SAIC Company.			
161962	DOC.20030 723.0003	BSC (Bechtel SAIC Company) 2003. <i>In-Package Chemistry Abstraction</i> . ANL-EBS-MD-000037 REV 02. Las Vegas, Nevada: Bechtel SAIC Company.	entire	corroborating/ supporting	WF reports related to FEPs
166845	DOC.20031 222.0012	BSC (Bechtel SAIC Company) 2003. Waste Form and In-Drift Colloids-Associated Radionuclide Concentrations: Abstraction and Summary. MDL-EBS-PA-000004 REV 00 ICN 01. Las Vegas, Nevada: Bechtel SAIC Company.	entire	corroborating/ supporting	Identification of responsible input waste form model reports
166296	DOC.20031 215.0001	BSC (Bechtel SAIC Company) 2003. Total System Performance Assessment-License Application Methods and Approach. TDR-WIS- PA-000006 REV 00 ICN 01. Las Vegas, Nevada: Bechtel SAIC Company.	Figure 3.2-2	corroborating/ supporting	Logic schematic for FEPs identification
162200	DOC.20040 408.0001	BSC (Bechtel SAIC Company) 2004. FEPs Screening of Processes and Issues in Drip Shield and Waste Package Degradation. ANL-EBS-PA- 000002 REV 02. Las Vegas, Nevada: Bechtel SAIC Company.	FEP 2.1.03.10.0A	corroborating/ supporting	Analysis of clogging of waste package breached zones by corrosion products.
168782	DOC.20040 331.0002	BSC (Bechtel SAIC Company) 2004. Features, Events, and Processes in UZ Flow and Transport. ANL-NBS-MD-000001 REV 02. Las Vegas, Nevada: Bechtel SAIC Company.	Section 6.3.9	corroborating/ supporting	UZ FEPs document; atmospheric transport of gases FEP discussion.
167461	DOC.20040 212.0004	BSC (Bechtel SAIC Company) 2004. Engineered Section 6.10 Barrier System: Physical and Chemical Environment Model. ANL-EBS-MD-000033 REV 02. Las Vegas, Nevada: Bechtel SAIC Company.	Section 6.10	corroborating/ supporting	Repository dust on the top of the waste packages is composed of non-corrosive minerals.
165923	DOC.20031 022.0001.	BSC 2003. <i>Dike/Drift Interactions</i> . MDL-MGR-GS-entire 000005 REV 00. Las Vegas, Nevada: Bechtel SAIC Company.	entire	corroborating/ supporting	Due to reactions and decreasing pressures, H <sub>2</sub> O, SO <sub>2</sub> and CO <sub>2</sub> released from the intrusion event will not make it to zone 2 in sufficient quantities to effect waste packages and waste forms in Zone 2 emplacement drifts.
167654	MOL.20040 414.0095	BSC 2004. Igneous Intrusion Impacts on Waste Packages and Waste Forms. MDL-EBS-GS-	Sections 5.4 and 6.5.2.2	corroborating/ supporting	Corrosive gases released during dike intrusion will not enter Zone 2 emplacement drifts in

Table 6-1. Supporting Information for Waste-Form FEPs Disposition (Continued)

DIRS	Accession or TIC number	Reference	Used From	Type of Information	Description
		000002 REV 01D. Las Vegas, Nevada: Bechtel SAIC Company.			sufficient quantities to effect waste packages and waste forms.
168411	MOL.20040 202.0085.	Buck, E.C.; McNamara, B.K.; Douglas, M.; and Hanson, B.D. 2003. Possible Incorporation of Neptunium in Uranyl (VI) Alteration Phases. PNNL-14277. Richland, Washington: Pacific Northwest National Laboratory.	entire	corroborating/ supporting	Np is incorporated into uranium-based alteration phases in approximately the same concentrations as presented in the mother solutions.
100388	240702	Buck, E.C.; Finch, R.J.; Finn, P.A.; and Bates, J.K. 1998. "Retention of Neptunium in Uranyl Alteration Phases Formed During Spent Fuel Corrosion." <i>Scientific Basis for Nuclear Waste Management XXI</i> , <i>Symposium held September 28-October 3, 1997, Davos, Switzerland</i> . McKinley, I.G. and McCombie, C., eds. <i>506</i> , 87-94. Warrendale, Pennsylvania: Materials Research Society.	entire	supporting/ supporting	Examination of corrosion products from spent fuel drip tests by electron energy loss spectroscopy (EELS) analyses in a transmission electron microscope.
100389	235501	Burns, P.C.; Ewing, R.C.; and Miller, M.L. 1997. "Incorporation Mechanisms of Actinide Elements into the Structures of U <sup>6+</sup> Phases Formed During the Oxidation of Spent Nuclear Fuel." <i>Journal of Nuclear Materials</i> , 245, ([1]), 1-9. Amsterdam, The Netherlands: North-Holland.	entire	corroborating/ supporting	Prediction that the substitutions Pu6+ in U6+ and (Np5+, Pu5+)in U6+ are likely to occur in most U6+ structures based on an analysis of the crystal-chemical properties of the U-O bond, Np-O bond, and Pu-O bond.
166275	DOC.20031 222.0006	Canori, G.F. and Leitner, M.M. 2003. <i>Project Requirements Document</i> . TER-MGR-MD-000001 REV 02. Las Vegas, Nevada: Bechtel SAIC Company.	entire	corroborating/ supporting	Project requirements document
161997	247873	Chen, Y. 2001. "An Empirical Np Solubility Model Based on Spent Fuel Dissolution Experiments." "Back to the Future - Managing the Back End of the Nuclear Fuel Cycle to Create a More Secure Energy Future," Proceedings of the 9th International High-Level Radioactive Waste Management Conference (IHLRWM), Las Vegas, Nevada, April 29-May 3, 2001. La Grange Park, Illinois: American Nuclear Society.	entire	supporting/ supporting	Analyses of the relative release rates of neptunium and uranium in the fuel degradation experiments in support of a close correlation between neptunium and uranium concentrations in the leachates.
162709	254363	Chen, Y. 2003. "Using Reactive Transport Modeling to Evaluate the Source Term at Yucca	pp. 385-397	corroborating/ supporting	Analyses of the relative release rates of neptunium and uranium in the fuel degradation

Table 6-1. Supporting Information for Waste-Form FEPs Disposition (Continued)

DIRS	Accession or TIC number	Reference	Used From	Type of Information	Description
		Mountain." Computers & Geosciences, 29, ([3]), 385-397. [New York, New York]: Pergamon.			experiments in support of a close correlation between neptunium and uranium concentrations in the leachates
161996	248663	Chen, Y.; Loch, A.R.; Wolery, T.J.; Steinborn, T.L.; Brady, P.V.; and Stockman, C.T. 2002. "Solubility Evaluation for Yucca Mountain TSPA-SR." <i>Scientific Basis for Nuclear Waste Management XXV</i> , Symposium held November 26-29, 2001, Boston, Massachusetts. McGrail, B.P. and Cragnolino, G.A., eds. 713, 775-782. Warrendale, Pennsylvania: Materials Research Society.	pp.775-782	supporting/ supporting	Analyses of the relative release rates of neptunium and uranium in the fuel degradation experiments in support of a close correlation between neptunium and uranium concentrations in the leachates
145441	246426	; Siegmann, E.; Mattie, P.; NcNeish, J.; an, S.D.; and Andrews, R. 1999. "A stic Model of Spent Fuel Dissolution, and Mineral Precipitation, and Np." Scientific Basis for Nuclear Wastement XXII, Symposium held November mber 4, 1998, Boston, Massachusetts, Nronkiewicz, D.J. and Lee, J.H., eds478. Warrendale, Pennsylvania: s Research Society.	pp. 471-488	supporting/	Analyses of the relative release rates of neptunium and uranium in the fuel degradation experiments in support of a close correlation between neptunium and uranium concentrations in the leachates
142613	225504	Croff, A.G. 1980. A User's Manual for the ORIGEN2 Computer Code. ORNL/TM-7175. Oak Ridge, Tennessee: Oak Ridge National Laboratory.	entire	corroborating/ supporting	Radionuclide inventory calculational code
101554	NNA.19910 326.0094	Croff, A.G. 1980. ORIGEN2 - A Revised and Updated Version of the Oak Ridge Isotope Generation and Depletion Code. ORNL-5621. Oak Ridge, Tennessee: Oak Ridge National Laboratory.	entire	corroborating/ supporting	Radionuclide inventory values
100264	MOL.19971 006.0075	CRWMS M&O 1997. <i>Waste Package Design Basis Events</i> . BBA000000-01717-0200-00037 REV 00. Las Vegas, Nevada: CRWMS M&O.	section 7.2.2.7, Table 7.2.2.7-1	corroborating/ supporting	Release of radioactive gases to the interior of the waste package will be too low to compromise waste package integrity.
100362	MOL.19981 008.0006	CRWMS M&O 1998. "Waste Form Degradation, Table 5-1 Radionuclide Mobilization, and Transport Through Figure 5-1 the Engineered Barrier System." Chapter 6 of	and	corroborating/ supporting	EDA-II design factors used in thermal analysis

Table 6-1. Supporting Information for Waste-Form FEPs Disposition (Continued)

DIRS Number	Accession or TIC number	Reference	Used From	Type of Information	Description
		Total System Performance Assessment-Viability Assessment (TSPA-VA) Analyses Technical Basis Document. B00000000-01717-4301-00006 REV 01. Las Vegas, Nevada: CRWMS M&O.			
			Page A6-29 Figure corroborating/ A6-1 supporting	corroborating/ supporting	Dissolution Rates for High-Level Waste, Metallic Carbide, and Ceramic Spent Nuclear Fuel
			entire	corroborating/ supporting	Support for mechanistic neptunium reactivity- transport model
			Table 5-1 and Figure 5-1	corroborating/ supporting	Support for judgement that preferential condensation will not be important.
105649	MOL.19981 217.0112	CRWMS M&O 1998. Immobilized in Ceramic. Volume II of Report on Intact and Degraded Criticality for Selected Plutonium Waste Forms in a Geologic Repository. BBA000000-01717-5705-00020 REV 01. Las Vegas, Nevada: CRWMS M&O.	entire	corroborating/ supporting	Support for the conclusion that DSNF codisposal and high-level radioactive waste glass waste packages are expected to be generally cooler than commercial SNF packages at the time of disposal for an approximate waste package center-to-center separation distance of ~5 m.
100374	MOL.19980 804.0099	CRWMS M&O 1998. Waste Form Degradation and Radionuclide Mobilization Expert Elicitation Project. Las Vegas, Nevada: CRWMS M&O.	entire	corroborating/ supporting	Radioactivity values in support of the conclusion that four radionuclides will dominate the total repository mass inventory (238U, 235U, 239Pu, and 236U).
103955	MOL.19990 528.0303	CRWMS M&O 1999. License Application Design Selection Report. B00000000-01717-4600-00123 REV 01. Las Vegas, Nevada: CRWMS M&O.	Section 4.4	corroborating/ supporting	Support for the conclusion that preferential condensation may not be important with the line loading of the EDA-II design
144128	MOL.20000 526.0336	CRWMS M&O 2000. Design Analysis for UCF Waste Packages. ANL-UDC-MD-000001 REV 00. Las Vegas, Nevada: CRWMS M&O.	entire	corroborating/ supporting	Investigation of the sensitivity of internal waste package pressures presuming fuel rods rupture, causing release of gases from the fuel matrix to the waste package interior
147651	MOL.20000 227.0240	CRWMS M&O 2000. Evaluation of Codisposal Executive Viability for HEU Oxide (Shippingport PWR) DOE-Summary Owned Fuel. TDR-EDC-NU-000003 REV 00. Las Vegas, Nevada: CRWMS M&O.		corroborating/ supporting	Characteristics of DOE spent fuel; HEU SNF
147650	MOL.20000 207.0689	CRWMS M&O 2000. Evaluation of Codisposal Viability for UZrH (TRIGA) DOE-Owned Fuel. TDR-EDC-NU-000001 REV 00. Las Vegas, Nevada: CRWMS M&O.	Executive	corroborating/ supporting	characteristics of DOE spent fuels; UZrH

Table 6-1. Supporting Information for Waste-Form FEPs Disposition (Continued)

DIRS Number	Accession or TIC number	Reference	Used From	Type of Information	Description
151561	MOL.20001 213.0066	CRWMS M&O 2000. <i>In-Drift Microbial</i> Communities. ANL-EBS-MD-000038 REV 00 ICN 01. Las Vegas, Nevada: CRWMS M&O.	entire	corroborating/ supporting	Microbial respiration is potentially able to increase in-drift $\text{CO}_2$ production by two orders of magnitude.
			Section 6.3 and 7.2 corroborating/ supporting	corroborating/ supporting	Potential sources for the release of gases from the fuel matrix to the waste package interior.
151659	MOL.20001 002.0145	CRWMS M&O 2000. Initial Cladding Condition. ANL-EBS-MD-000048 REV 00 ICN 01. Las Vegas, Nevada: CRWMS M&O.	Section 6.3.3	corroborating/ supporting	Fission and radioactive-gas diffusion rates
153595	MOL.20010 103.0211	CRWMS M&O 2000. Relative Contribution of Individual Radionuclides to Inhalation and Ingestion Dose. CAL-WIS-MD-000002 REV 00. Las Vegas, Nevada: CRWMS M&O.	entire	corroborating/ supporting	Support for the conclusion that the DSNF codisposal and high-level radioactive waste glass waste packages are expected to be generally cooler
			entire	corroborating/ supporting	Support for the contention that omission of DSNF cladding degradation as a system-wide feature from the performance assessment models will not significantly change the interpretation of expected dose
151940	MOL.20000 831.0280	CRWMS M&O 2000. Unsaturated Zone Flow and Sections 3.3, 3.6 Transport Model Process Model Report. TDR-NBS-HS-000002 REV 00 ICN 02. Las Vegas, Nevada: CRWMS M&O.		corroborating/ supporting	Support for the conclusion that any gas produced in the repository will tend to flow through the fracture complex with some gas diverted to the matrix at unit interfaces or where fracture networks pinch out. These flow paths will disperse flammable gas concentrations to levels below the ignition point.
118968	248046	DOE (U.S. Department of Energy) 2000. DOE Spent Nuclear Fuel Grouping in Support of Criticality, DBE, TSPA-LA. DOE/SNF/REP-0046, Rev. 0. Idaho Falls, Idaho: U.S. Department of Energy, Idaho Operations Office.	entire	corroborating/ supporting	Classification of DSNF types
149432	247664	DOE (U.S. Department of Energy) 1997.  EM/RW Repository Task Team Report: Grouping Method to Minimize Testing for Repository Emplacement of DOE SNF. DOE/SNF/REP-008, Rev. 0. Idaho Falls, Idaho: U.S. Department of Energy.	pp. 20-21	corroborating/ supporting	Potential for pyrophoric reactions: oxide fuels, metal fuels, and carbide fuels.

Table 6-1. Supporting Information for Waste-Form FEPs Disposition (Continued)

DIRS	Accession or TIC number	Reference	Used From	Type of Information	Description
			page 21	corroborating/ supporting	Uranium-metal spent fuel is more chemically reactive than other spent fuel.
100550	MOL.19981 007.0030	DOE (U.S. Department of Energy) 1998. Total System Performance Assessment. Volume 3 of Viability Assessment of a Repository at Yucca Mountain. DOE/RW-0508. Washington, D.C.: U.S. Department of Energy, Office of Civilian Radioactive Waste Management.	Sections 3.5.3 and 5.5.3	corroborating/ supporting	HLW glass is not a major contributor to total activity.
122980	243859	DOE (U.S. Department of Energy) 1998. Update Appendix A, to Assessment of Product Output Disposal in Unsaturated Tuff of Spent Nuclear Fuel and High-Level Waste Owned by U.S. Department of Energy. DOE/SNF/REP-015. Washington, D.C.:	Appendix A, Section 6.9, p. 41	corroborating/ supporting	Broken Peach-Bottom Core-1 pellets have an estimated cladding failure rate of 35%
			Table 1-1, p.1-8 and Appendix B, p. 14	corroborating/ supporting	1.663 MTHM of Peach Bottom Core 1 pellets contained in 103 waste packages, will be disposed in the repository.
			Appendix B, p. 14 and Table 1-1, p.1-8	corroborating/ supporting	24.667 MTHM of high-integrity fuel (contained in 545 waste packages) from the Fort St. Vrain and Peach-Bottom Core 2 reactors
			entire	corroborating/ supporting	HLW glass will constitute a large volume fraction of the total volume of waste in the repository
158873	MOL.20020 326.0056	DOE 2002. Waste Acceptance System Requirements Document. DOE/RW-0351, REV 4.3.1.B, 4.3 04. Washington D.C.: U.S. Department of Energy, and 4.3.17 Office of Civilian Radioactive Waste Management.	Section 4.2.11, 4.3.1.B, 4.3.7.B, and 4.3.17	corroborating/ supporting	Restriction on organic and chemically reactive materails in the waste canisters emplaced in the repository
158405	252089	DOE (U.S. Department of Energy) 2002 DOE Spent Nuclear Fuel Information in Support of TSPA-SR. DOE/SNF/REP-0047, Rev. 2. [Washington, D.C.; U.S. Department of Energy, Office of Environmental Management.	Section 1 and Appendix D	supporting/ supporting	The only fuel waste capable of producing flammable gasses is U/Th carbide DSNF waste. Only a small fraction(~1%) of the DSNF fuel contains U/Th carbide. Since the carbide spent fuels will amount to less than 0.04% of the waste packages, and all DNSF waste will be widely dispersed throughout the repository, any flammable gas produced will be widely dispersed.

Table 6-1. Supporting Information for Waste-Form FEPs Disposition (Continued)

DIRS Number	Accession or TIC number	Reference	Used From	Type of Information	Description
			entire	corroborating/ supporting	Characteristics of DSNF waste to be disposed in the repository.
162004	MOL.20031 119.0180.	Finch, R.J. and Fortner, J.A. 2002. Dissolved Concentration Limits: Neptunium in Alteration Phases, A Progress Report. Argonne, Illinois: Argonne National Laboratory.	entire	corroborating/ supporting	Analysis of dissolved concentrations of radioactive elements which includes high carbon dioxide partial pressures.
161979	248663	Finch, R.J.; Fortner, J.A.; Buck, E.C.; and Wolf, S.F. 2002. "Neptunium Incorporation into Uranium(VI) Compounds Formed During Aqueous Corrosion of Neptunium-Bearing Uranium Oxides." Scientific Basis for Nuclear Waste Management XXV, Symposium held November 26-29, 2001, Boston, Massachusetts. McGrail, B.P. and Cragnolino, G.A., eds. 713, 647-654. Warrendale, Pennsylvania: Materials Research Society.	Section 6	corroborating/ supporting	Experimental results on neptunium incorporation into dehydrated schoepite and estimated that the amount of neptunium incorporated in dehydrated schoepite can be as high as 2 percent of the host solid based on EELS measurement.
144061	247586	Foster, A.R. and Wright, R.L., Jr. 1973. <i>Basic Nuclear Engineering.</i> 2nd Edition. Boston, Massachusetts: Allyn and Bacon.	p. 296-297	corroborating/ supporting	Basic Nuclear Engineering textbook - it requires a minimum displacement energy, Ed, of approximately 25 ev to eject the struck atom from its lattice site. displacement of atoms corresponds to a threshold event, P(T) is modeled as a Heaviside step function.
163911	MOL.20030 617.0128	Friese, J.I. 2003. "Transmittal of Draft Version of Existing Evidence for the Fate of Neptunium in the Yucca Mountain Repository, Pacific Northwest National Laboratory." Interoffice memorandum from J.I. Friese (BSC) to Y. Chen, June 17, 2003, 0613037658, with attachment.	entire	corroborating/ supporting	Draft Input - Existing Evidence for the Fate of Neptunium in the Yucca Mountain Repository.
162634	MOL.20040 303.0023	Friese, J.I.; Buck, E.C.; McNamara, B.K.; Hanson, B.D.; and Marschman, S.C. 2003. <i>Existing Evidence for the Fate of Neptunium in the Yucca Mountain Repository.</i> PNNL-14307. Richland, Washington: Pacific Northwest National Laboratory.	Entire	corroborating/ supporting	Distribution of neptunium in the repository.
168471	HQX.19881 021.0025	Gray, W.J. 1988. Effect of Surface Oxidation, Alpha Radiolysis, and Salt Brine Composition on	entire	corroborating/ supporting	Laboratory experiments show little efffect of alpha radiolysis on the leaching behavior of

Table 6-1. Supporting Information for Waste-Form FEPs Disposition (Continued)

DIRS Number	Accession or TIC number	Reference	Used From	Type of Information	Description
		Spent Fuel and UO2 Leaching Performance. PNL/SRP-6689. Richland, Washington: Pacific Northwest Laboratory.			spent fuel and UO2 samples.
109691	245380	Gray, W.J. and Einziger, R.E. 1998. <i>Initial</i> Results from Dissolution Rate Testing of N- Reactor Spent Fuel Over a Range of Potential Geologic Repository Aqueous Conditions. DOE/SNF/REP-022, Rev. 0. Washington, D.C.: U.S. Department of Energy.	Section 4	corroborating/ supporting	Rapid corrosion rate of the metallic uranium uranium that is the matrix of N-Reactor SSNF compared with other SNF
149367	247872	Kaplan, I. 1963. <i>Nuclear Physics</i> . 2nd edition. Reading, Massachusetts: Addison-Wesley Publishing.	p. 307	corroborating/ supporting	Commercial fuel cladding will remain intact and should substantially reduce alpha dose rates to groundwater
152482	248909	Lam, P.S.; Sindelar, R.L.; and Peacock, H.B. Jr. 1997. Vapor Corrosion of Aluminum Cladding Alloys and Aluminum-Uranium Fuel Materials in Storage Environments (U). WSRC-TR-97-0120. Aiken, South Carolina: Westinghouse Savannah River Company.	Section 8	corroborating/ supporting	Aluminum-clad uranium metal DSNF does not have the amount of damage/corrosion (and consequent extent of hydriding and potential for pyrophoricity) nor the propensity to form uranium hydrides as a result of corrosion, shown by the N-Reactor SNF
168475	MOL.20040 325.0053	Lawrence, L.A. 1999. <i>K Basin Spent Nuclear Fuel</i> Section 5.1 and <i>Characterization</i> . HNF-3534, Rev. 0. Richland, Table 1 Washington: Duke Engineering & Services Hanford, Inc.		corroborating/ supporting	Estimate of approximately 33% (by means of visual survey) for the fraction of failed N-Reactor spent fuel assemblies for both the K-East and K-West basins.
142133	243883	Lederer, C.M. and Shirley, V.S., eds. 1978. <i>Table of Isotopes</i> . 7th Edition. New York, New York: John Wiley & Sons.	p. 1464	corroborating/ supporting	Table of isotopes
149429	248059	Marschman, S.C.; Pyecha, T.D.; and Abrefah, J. 1997. <i>Metallographic Examination of Damaged N</i> Reactor Spent Nuclear Fuel Element SFEC5,4378. PNNL-11438. Richland, Washington: Pacific Northwest National Laboratory.	Section 3.4.2	corroborating/ supporting	Uranium hydride inclusions tend to be concentrated near the exposed uranium metal fuel surface of damaged N-Reactor SNF
158010	MOL.20020 404.0085	McKenzie, D.G., IV. 2002. Waste Package Design Methodology Report. TDR-MGR-MD- 000006 REV 02. Las Vegas, Nevada: Bechtel SAIC Company.	entire	corroborating/ supporting	Waste package and EBS design description.

Table 6-1. Supporting Information for Waste-Form FEPs Disposition (Continued)

DIRS Number	Accession or TIC number	Reference	Used From	Type of Information	Description
164527		MO0307SEPFEPS4.000. LA FEP List. Submittal entire date: 07/31/2003.	entire	corroborating/ supporting	LA FEP list
163274	254568	NRC (U.S. Nuclear Regulatory Commission) 2003. <i>Yucca Mountain Review Plan, Final Report</i> . NUREG-1804, Rev. 2. Washington, D.C.: U.S. Nuclear Regulatory Commission, Office of Nuclear Material Safety and Safeguards.	Section 2.2.1.2	corroborating/ supporting	Yucca Mountain Review Plan for screening FEPs
103896	233705	Parrington, J.R.; Knox, H.D.; Breneman, S.L.; Baum, E.M.; and Feiner, F. 1996. <i>Nuclides and Isotopes, Chart of the Nuclides</i> . 15th Edition. San Jose, California: General Electric Company and KAPL, Inc.	p.8	corroborating/ supporting	Many of the heavy radionuclides emit alpha particles with energies greater than 4.0 MeV
			entire	corroborating/ supporting	significant portion of the radionuclides in the expected YMP inventory are alpha emitters.
149395	247663	Propp, W.A. 1998. <i>Graphite Oxidation Thermodynamics/Reactions</i> . DOE/SNF/REP- 018, Rev. 0. Idaho Falls, Idaho: U.S. Department of Energy.	enntire	corroborating/ supporting	that hydrocarbon production is not a problem with carbide fuels
161925	252663	Quinones, J.; Grambow, B.; Loida, A.; and Geckeis, H. 1996. "Coprecipitation Phenomena During Spent Fuel Dissolution. Part 1: Experimental Procedure and Initial Results on Trivalent Ion Behaviour." <i>Journal of Nuclear Materials</i> , 238, [[1]), 38-43. Amsterdam, The Netherlands: Elsevier.	pp. 38-43	corroborating/ supporting	Support for the conclusion that the large discrepancy in Np solubility is due to the incorporation of actinides into secondary uranium phases, that was not accounted for in conventional solubility calculations.
101084	237102	Rechard, R.P., ed. 1995. <i>Methodology and Results</i> . Volume 2 of <i>Performance Assessment of the Direct Disposal in Unsaturated Tuff of Spent Nuclear Fuel and High-Level Waste Owned by U.S. Department of Energy.</i> SAND94-2563/2. Albuquerque, New Mexico: Sandia National Laboratories.	Section 11.3.1, p. 11-24)	corroborating/ supporting	Estimate of the amount of damaged cladding in DSNF. For approximately 80% of the DSNF that is N-Reactor SNF, the cladding will be significantly damaged at the time of emplacement in their canisters. Up to 50 percent may be already perforated
149433	247814	Reilly, M.A. 1998. Spent Nuclear Fuel Project Technical Databook. HNF-SD-SNF-TI-015, Rev. 5. Richland, Washington: Fluor Daniel Hanford.	p.30	corroborating/ supporting	It is possible that additional U-hydride will form in N-Reactor SNF during interim storage.

Table 6-1. Supporting Information for Waste-Form FEPs Disposition (Continued)

DIRS	Accession or TIC number	Reference	Used From	Type of Information	Description
149368	247643	Sanchez, L.C.; Rath, J.S.; Aguilar, R.; Trellue, H.R.; Cochrane, K.; Taylor, L.L.; and Wilson, J.R. 1998. <i>Nuclear Dynamics Consequence Analysis (NDCA) for the Disposal of Spent Nuclear Fuel in an Underground Geologic Repository.</i> DOE/SNF/REP-0033, REV 0. Three Volumes. Washington, D.C.: U.S. Department of Energy.	entire	corroborating/ supporting	Radionuclide inventories for final waste forms
159406	243079	<i>of</i> ord.	entire	corroborating/ supporting	Description and analysis of the pyrophoric behavior of N-Reactor SNF during reprocessing operations.
113368	246431	Shoesmith, D.W. and Sunder, S. 1992. "The Prediction of Nuclear Fuel (UO2) Dissolution Rates Under Waste Disposal Conditions." <i>Journal of Nuclear Materials, 190,</i> 20-35. Amsterdam, The Netherlands: Elsevier.	entire	corroborating/ supporting	Support for the conclusion that water will not intrude until gamma and beta emitters have decayed to very low concentrations
166960	DOC.20040 120.0004	Simmons, A.M. 2004. Yucca Mountain Site Description. TDR-CRW-GS-000001 REV 02. Two volumes. Las Vegas, Nevada: Bechtel SAIC Company.	Section 7.9.1.8	corroborating/ supporting	Description of gas flow in the unsaturated zone.
165881	103316	Solbrig, C.W.; Krsul, J.R.; and Olsen, D.N. 1994. "Pyrophoricity of Uranium in Long-Term Storage Environments." <i>Proceedings of the Topical Meeting on DOE Spent Nuclear Fuel-Challenges and Initiatives, Salt Lake City, Utah, December 13-16, 1994.</i> Pages 89-93. La Grange Park, Illinois: American Nuclear Society.	pp 89-93	corroborating/ supporting	Description of two pyrophoric events concerning uranium metal-based nuclear fuel.
143815	246920	Sunder, S. and Shoesmith, D.W. 1991.  Chemistry of UO <sub>2</sub> Fuel Dissolution in Relation to the Disposal of Used Nuclear Fuel. AECL-10395. Pinawa, Manitoba, Canada: Whiteshell Laboratories, Atomic Energy of Canada Limited.	entire	corroborating/ supporting	Support for the conclusion that water will not intrude (i.e., the waste container will not fail) until gamma and beta emitters have decayed to very low concentrations, and that strong gamma and beta fields associated with the used fuel will decrease by a factor >103 in the first few hundred years after disposal.
143860	246914	Sunder, S.; Shoesmith, D.W.; and Miller, N.H. 1997. "Oxidation and Dissolution of Nuclear Fuel (UO <sub>2</sub> ) by the Products of the Alpha Radiolysis of	p. 67	corroborating/ supporting	Radiation fields decrease dramatically over the first 1,000 years after the fuel is out-of-reactor

Table 6-1. Supporting Information for Waste-Form FEPs Disposition (Continued)

DIRS Number	Accession or TIC number	Reference	Used From	Type of Information	Description
		Water." <i>Journal of Nuclear Materials, 244,</i> 66-74. Amsterdam, The Netherlands: Elsevier.			
168468	MOL.20040 325.0049	Swanson, J.L.; Bray, L.A Kjarmo, H.E.; Ryan, J.L.; Matsuzaki, C.L.; Pitman, S.G.; Haberman, J.H. Laboratory Studies of Shear/Leach Processing of Zircaloy Clad Metallic Uranium Reactor Fuel. PNL-5708, December 1985.	Sections 7. and 10.	corroborating/ supporting	Analysis of the cause of the ignition and burning of sheared metallic uranium spent fuel elements in the dissolvers at West Valley. The most probable cause for the ignition was concluded to be the sensitization of fuel element weld beads by the very acidic dissolver solutions
125082	MOL.19981 019.0001	Thornton, T.A. 1998. "HPPP Issue 1; Preliminary TSPA for a Pyrophoric Event Involving N-Reactor SNF Waste Packages." Interoffice correspondence from T.A. Thornton (CRWMS M&O) to J.S. Clouet, S.S. Sareen, and D. Stahl, September 21, 1998, LV.WP.TAT.09/98-	entire	corroborating/ supporting	Support for the conclusion that overall repository performance is very insensitive to the DSNF degradation rate
107796	MOL.19980 730.0142	Thornton, T.A. 1998. "HPPP Issue 1; Preliminary TSPA for N-Reactor SNF Waste Packages." Interoffice correspondence from T.A. Thornton (CRWMS M&O) to J.S. Clouet, S.S. Sareen, and D. Stahl, June 1, 1998, LV.WP.TAT.05/98-111, with attachment.	entire	corroborating/ supporting	DSNF contribution to postclosure dose is negligible
113466	243085	Werme, L.O. and Spahiu, K. 1998. "Direct Disposal of Spent Nuclear Fuel: Comparison Between Experimental and Modelled Actinide Solubiluties in Natural Waters." Journal of Alloys and Compounds, 271-273, 194-200. Lausanne, Switzerland: Elsevier.	pp. 194-200	corroborating/ supporting	Support for the conclusion that the large discrepancy in Np solubility is due to the incorporation of actinides into secondary uranium phases, that was not accounted for in conventional solubility calculations.
143651	248002	Wick, O.J., ed. 1980. Plutonium Handbook: A Guide to the Technology. Volumes I & II. La Grange Park, Illinois: American Nuclear Society.	Section 7.1	corroborating/ supporting	Density of pure plutonium metal
100191	NNA.19940 112.0123	Wilson, M.L.; Gauthier, J.H.; Barnard, R.W.; Barr, G.E.; Dockery, H.A.; Dunn, E.; Eaton, R.R.; Guerin, D.C.; Lu, N.; Martinez, M.J.; Nilson, R.; Rautman, C.A.; Robey, T.H.; Ross, B.; Ryder, E.E.; Schenker, A.R.; Shannon, S.A.; Skinner, L.H.; Halsey, W.G.; Gansemer, J.D.; Lewis, L.C.; Lamont, A.D.; Triay, I.R.; Meijer, A.; and Morris,	entire	corroborating/ supporting	Radionuclide inventory values

Table 6-1. Supporting Information for Waste-Form FEPs Disposition (Continued)

DIRS Number	Accession or TIC number	Reference	Used From	Type of Information	Description
		D.E. 1994. Total-System Performance Assessment for Yucca Mountain – SNL Second Iteration (TSPA-1993). SAND93-2675. Executive Summary and two volumes. Albuquerque, New Mexico: Sandia National Laboratories.			
165884	255359	Wood, D.; Snowden, S.; Howe Jr, H.; Thomas, L.; pp. 113-115 Moon, D.; Gregg, H.; Miller, P. 1994. "Regarding the chemistry of metallic uranium stored in steel drums." <i>Journal of Nuclear Materials</i> , 209, 113-115. New York, New York: Elsevier.	pp. 113-115	corroborating/ supporting	corroborating/ Description of a prophoric event concerning supporting metallic uranium fuel elements.
156713	MOL.20010 322.049, MOL.20011 107.0002	MOL.20010 YMP (Yucca Mountain Site Characterization 322.049, Project) 2001. Yucca Mountain Site MOL.20011 Characterization Project Requirements Document (YMP-RD). YMP/CM-0025, Rev. 4, DCN 02. Las Vegas, Nevada: Yucca Mountain Site Characterization Office.	Table 1.3-1 and p. 1.3-6	corroborating/ supporting	Table 1.3-1 and p. corroborating/ Relative amounts of CSNF,HLW glass, and 1.3-6 aupporting DSNF to be disposed in the repository.

#### 6.1 APPROACHES

The NRC requires consideration and evaluation of FEPs as part of the performance assessment activities. More specifically, NRC regulations allow the exclusion of FEPs from the TSPA if they can be shown to be of low probability or of low consequence. The specified criteria can be summarized in the form of two FEP screening statements as follows.

- 1. The event has at least one chance in 10,000 of occurring over 10,000 years (see 10 CFR 63.114(d) [DIRS 156605]).
- 2. The magnitude and time of the resulting radiological exposure to the RMEI, or radionuclide release to the accessible environment, would be significantly changed by its omission (see 10 CFR 63.114 (e and f) [DIRS 156605]).

Additionally, the acceptance criteria in *Yucca Mountain Review Plan, Final Report* (NRC 2003 [DIRS 163274], Section 2.2.1.2.1.3) calls for evaluating the FEPs based on the regulations. This criterion can be summarized in the form of a third FEP screening statement.

3. The FEP is not excluded by regulation.

If there are affirmative conditions for all three screening criteria, the FEP is "included" in the TSPA-LA model. If there is a negating condition in any of the three screening criteria, the FEP is "excluded" from the TSPA-LA model.

Evaluation of the FEPs against these screening statements may be done in any order. In practice, by-regulation criteria were examined first, and then either low probability or low consequence criteria were examined. FEPs that were retained on one criterion (e.g., regulatory guidance) were also considered against the other criteria (probability and consequence). Consequently, the application of the analyst's judgment regarding the order in which to apply the criteria does not affect the final decision. Allowing the analyst to choose the most appropriate order to apply the criteria prevents needless work, such as developing quantitative probability arguments for low-consequence events or complex consequence models for low-probability events.

Regardless of the specific approach chosen to perform the screening, the screening process is in essence a comparison of the FEP against the criteria specified in Section 4.2. The outcome of the screening is independent of the particular methodology selected to perform the screening.

Alternative interpretations of data as they pertain directly to the FEPs screening are provided in the sections for each FEP, as discussed below. The FEPs screening decisions may also rely on the results of analyses performed and documented as separate activities. Alternative approaches related to separate activities and analyses are addressed in the specific analysis model reports for those analyses and are not discussed in this report.

#### 6.2 WASTE-FORM FEPS SCREENING AND ANALYSES

This section addresses the 41 waste-form FEPs identified for TSPA-LA (see Section 1.2.1 and Table 1.2-1). Each FEP is screened for inclusion or exclusion in TSPA-LA, using the criteria outlined in Section 4.2.1 based on requirements defined by the NRC (10 CFR 63.114(d)(e)(f) [DIRS 156605]).

The screening decisions, screening arguments, and TSPA dispositions for the waste-form FEPs in some cases reference and utilize model reports or analysis reports currently in process or for which there are planned ICNs. If the final version of these model reports and analysis reports are inconsistent with the analyses in this report, this report will be modified per the AP-SIII.9Q checking and review process and per the requirements of the controlled version of the technical work plan at the time of the revisions.

## **6.2.1** Igneous Intrusion Interacts with EBS Components

#### **FEP Number:**

1.2.04.04.0A

**FEP Description**: An igneous intrusion in the form of a dike occurs through the repository, intersecting the repository drifts. Magma, pyroclastics, and volcanic gases enter the drift and interact with the EBS components including drip shields, waste packages, pallet, and invert. This leads to accelerated drip shield and waste package failure (e.g. attack by magmatic volatiles, damage by flowing or fragmented magma, or thermal effects) and dissolution or volatilization of waste.

#### **Descriptor Phrases:**

Igneous intrusion (drip shield damage)
Igneous intrusion (waste package damage)
Igneous intrusion (cladding damage)
Chemical effects of igneous intrusion in EBS (solubility)
Thermal effects of igneous intrusion in EBS

# **Screening Decision:**

Included

# **Screening Argument:**

N/A

**TSPA Disposition**: The effects of an igneous intrusion into the repository are implemented in the TSPA through the delineation of two zones. Zone 1 encompasses portions of the drifts where EBS components are directly contacted by magma. Zone 2 encompasses the remainder of the drifts, where EBS components are not contacted by magma, but are exposed to high temperature and magmatic gases. Details of how an igneous intrusion interacts with EBS components is described in *Igneous Intrusion Impacts on Waste Packages and Waste Forms* (BSC 2004 [DIRS 167654]. A summary of the effects of igneous intrusion is presented here.

### Damage and Thermal Effects in Zone 1

Igneous Intrusion Impacts on Waste Packages and Waste Forms (BSC 2004 [DIRS 167654], Section 6.5.1) indicates the igneous intrusion would render the drip shields, waste packages, and cladding in the Zone 1 emplacement drifts ineffective so they would provide no further protection to the waste. The exposed waste form would then be distributed throughout the cooled magma, though exactly how is unknown (Section 5.2.1 of this analysis report). Spent fuel is a refractory material and considered to be chemically unaffected by exposure to the intruding

magma. Likewise, waste glass degradation behavior is considered likely to be minimally affected by any consequent devitrification (BSC 2004 [DIRS 167619], Section 7.5.4). As the waste forms will be distributed throughout the magma body, the temperature of those waste forms can be considered the same as the temperature of the cooling magma. These values are presented in DTN: MO0402SPAHWCIG.002 [DIRS 168762].

## Damage and Thermal Effects in Zone 2

The impacts of magmatic heat conduction from Zone 1 to Zone 2 emplacement drifts were modeled by numerical simulations of nonsteady state heat conduction with radial flow in *Igneous Intrusion Impacts on Waste Packages and Waste Forms* (BSC 2004 [DIRS 167654], Section 6.5.2.1 and Attachment I). The simulation modeling of heat conduction away from the intruded drifts demonstrates that the initial 1,150°C temperature reduces to about 30°C at the center of the drift in about 30 years, and the maximum temperature rise expected in the Zone 2 emplacement drifts is less than 1°C. The drift-rock in Zone 2 provides an effective thermal insulation barrier to the impacts of high temperature of intruded magma and there would not be any impact of igneous heat on the waste packages, drip shield, or cladding in Zone 2 emplacement drifts.

An analysis of gas flow from Zone 1 to Zone 2 emplacement drifts is detailed in *Dike/Drift Interactions* (BSC 2003 [DIRS 165923]). This report shows that due to reactions and decreasing pressures, H<sub>2</sub>O, SO<sub>2</sub> and CO<sub>2</sub> released from the intrusion event will not make it to Zone 2 in sufficient quantities to affect waste packages and waste forms in Zone 2 emplacement drifts. Effects of other corrosive gases is discussed in Sections 5.4 and 6.5.2.2 of *Igneous Intrusion Impacts on Waste Packages and Waste Forms* (BSC 2004 [DIRS 167654]). These sections also conclude that corrosive gases released during dike intrusion will not enter Zone 2 emplacement drifts in sufficient quantities to affect waste packages and waste forms.

#### **Chemical Effects**

After postintrusive magma cooling and reversion to normal in-drift environmental conditions, seepage water flowing through the intruded basalt will be chemically altered by reaction with basaltic minerals. As demonstrated in *Igneous Intrusion Impacts on Waste Packages and Waste Forms* (BSC 2004 [DIRS 167654]), this alteration involves significant changes to the pH and ionic strength of the solution. The pH and fCO<sub>2</sub> values obtained through reaction of seepage water with basalt should be used in conjunction with *Dissolved Concentration Limits of Radioactive Elements* (BSC 2003 [DIRS 163152]) to describe the solubility of the waste forms. Because waste forms are conservatively considered chemically unchanged (BSC 2004 [DIRS 167654], Section 6.5.1.2), the dissolved concentration of radioelements in water would have the same dependency on water chemistry in regions influenced by an igneous intrusion as those regions that are not. Thus, the solubility tables given in *Dissolved Concentration Limits of Radioactive Elements* (BSC 2003 [DIRS 163152]) should be used to determine concentrations of radionuclides in basalt-filled drifts the same way they are used in magma-free drifts.

## **Supporting Documents:**

BSC 2004 [DIRS 167654]

#### **Related FEPs:**

N/A

## **6.2.2** Waste Inventory

#### **FEP Number:**

2.1.01.01.0A

**FEP Description**: The waste inventory includes all potential sources of radiotoxicity and chemical toxicity. It consists of the radionuclide inventory (typically in units of curies), by specific isotope, of anticipated radionuclides in the waste, and the nonradionuclide inventory (typically in units of density or concentration) that consists of both physical, e.g., CSNF, DNSF, and HLW, and chemical waste constituents. The radionuclide composition of the waste will vary due to initial enrichment, burnup, the number of fuel assemblies per container, and the decay time subsequent to discharge of the fuel from the reactor.

Also consider that the fuel types, matrices, radionuclide mixes, and nonradionuclide inventories in DSNF and HLW may differ from CSNF. Additional waste types should be considered if they are proposed for disposal at Yucca Mountain.

## **Descriptor Phrases:**

Radionuclide inventory Nonradionuclide inventory CSNF inventory DSNF inventory HLW glass inventory Gap inventory

### **Screening Decision:**

Included

### **Screening Argument:**

N/A

**TSPA Disposition**: Modeling the waste inventory in TSPA-LA can be divided into two tasks. The first is to select those radionuclides important to dose calculations. The second is to determine which radionuclides are present in each type of waste and in what quantity.

The radionuclides of importance to dose calculations were assessed in *Radionuclide Screening* (BSC 2002 [DIRS 160059]). This information was provided to *Initial Radionuclide Inventories* (BSC 2003 [DIRS 161961]) and is reproduced in Table 13 of that report. The table presents those radionuclides relevant to the nominal, igneous disruption, and human intrusion scenario classes and further breaks down the list into the radionuclides of importance for the periods from 100 to 10,000 years (for TSPA-LA calculations) and from 10,000 to 1,000,000 years (for EIS calculations). Nonradioactive waste is not modeled. 20 radionuclides of interest were identified from the TSPA-LA screening. The separate groundwater protection standard required that <sup>228</sup>Ra be added to the list. The precursors of the screened-in radionuclides were also required, which added another seven radionuclides. As a result, 28 isotopes were modeled in the TSPA:

<sup>241</sup>Am, <sup>243</sup>Am, <sup>14</sup>C, <sup>245</sup>Cm, <sup>135</sup>Cs, <sup>137</sup>Cs, <sup>129</sup>I, <sup>237</sup>Np, <sup>231</sup>Pa, <sup>238</sup>Pu, <sup>239</sup>Pu, <sup>240</sup>Pu, <sup>241</sup>Pu, <sup>242</sup>Pu, <sup>226</sup>Ra, <sup>228</sup>Ra, <sup>90</sup>Sr, <sup>99</sup>Tc, <sup>229</sup>Th, <sup>230</sup>Th, <sup>232</sup>U, <sup>232</sup>U, <sup>233</sup>U, <sup>234</sup>U, <sup>235</sup>U, <sup>236</sup>U, and <sup>238</sup>U (BSC 2003 [DIRS 161961], Table 16). Four additional radionuclides were added to the inventory to retain the capability to do 1-million year EIS calculations: <sup>36</sup>Cl, <sup>210</sup>Pb, <sup>79</sup>Se, and <sup>126</sup>Sn (BSC 2003 [DIRS 161961], Table 16).

Nominal average inventories of radionuclides for each type of waste are documented in *Initial Radionuclide Inventories* (BSC 2003 [DIRS 161961]). In the analysis, three types of uncertainty are applied to the nominal inventories: computational methods and nuclear data, completeness of records, and future decisions. Application of these uncertainties resulted in weighted average grams per package for the 32 radionuclides and 3 waste types (CSNF, DSNF, and HLW). Table 21 of *Initial Radionuclide Inventories* (BSC 2003 [DIRS 161961]) lists these values. The CSNF inventory for <sup>14</sup>C includes minor contributions (18 percent) from activation of CSNF assembly hardware outside the cladding. Additional contributions from activated mineral deposits (crud) were found to be insignificant and were not considered as part of the inventory (BSC 2003 [DIRS 161961]).

The weighted average waste inventory values (grams per package for each radionuclide for each waste type) are input to GoldSim for use in the TSPA-LA model. The *Initial Radionuclide Inventories* (BSC 2003 [DIRS 161961]) also provides GoldSim with radionuclide decay rates. As the drip shield, waste package, cladding and waste form are subjected to degradation processes or disruptive events, the radionuclides can be mobilized and transported.

## **Supporting Documents:**

BSC 2003 [DIRS 161961]

#### **Related FEPs:**

- 3.1.01.01.0A, Radioactive decay and ingrowth
- 2.1.01.03.0A, Heterogeneity of waste inventory

### **6.2.3** Interactions between Colocated Waste

#### **FEP Number:**

2.1.01.02.0A

**FEP Description**: Colocation refers to the disposal of CSNF, DSNF, HLW, and possibly other wastes in close proximity within the repository. Colocation might affect thermal outputs, chemical interactions, or radionuclide mobilization.

#### **Descriptor Phrases:**

Colocated waste (chemical interactions between waste packages)

Colocated waste (thermal interactions, preferential condensation)

Other waste types (intermediate-level radioactive waste, low-level radioactive waste, and nonradioactive waste)

#### **Screening Decision:**

Excluded (low consequence)

**Screening Argument**: The following waste forms will be part of the initial license application submittal (BSC 2003 [DIRS 161961]):

- CSNF from boiling-water and pressurized-water reactors
- DSNF (including naval SNF), approximately 80 percent by weight of which is the N-Reactor SNF currently stored at Hanford
- HLW in the form of glass logs in stainless steel canisters.

Regulatory restrictions will prevent colocation of these waste forms with low- and intermediate-level nuclear waste, toxic chemical wastes, or wastes disposed by future human activity. These waste forms will be placed in specially designed waste packages with all of the HLW and some of the DSNF form designated for codisposal. Present plans call for five glass logs and one DSNF canister to be placed in each codisposal package (DOE 2002 [DIRS 158405], Section 9). The codisposal packages will be colocated randomly within an array comprised predominantly of CSNF waste packages, and will contain a relatively small fraction of the total waste.

The codisposal waste packages are expected to be generally cooler (CRWMS M&0 2000 [DIRS 147650]; CRWMS M&0 2000 [DIRS 147651]) than CSNF waste packages at the time of disposal. Preferential condensation due to this colocated waste could possibly occur under the dripshield just above the relatively cooler codisposal (DSNF and HLW) waste packages. Condensate droplets that would eventually fall, preferentially onto the codisposal waste packages, could increase glass degradation rates, DSNF clad degradation, and dissolution, thus releasing HLW-DSNF radionuclides. Preferential condensation may be less important with the line loading of the EDA-II design (CRWMS M&O 1999 [DIRS 103955], Table 5-3; CRWMS M&O 1998 [DIRS 100362], Table 5-1 and Figure 5-1), which is designed to keep the waste packages at nearly equal temperatures. Moreover, it was determined in Section 6.10 of Engineered Barrier System: Physical and Chemical Environment Model (BSC 2004 [DIRS 167461], Tables 6.10-7 and 6.10-8) that brines formed by deliquescence in the repository dust on the top of the waste packages have pH and water chemistry (particularly pH) characteristics that are not problematic for the codisposal waste forms. This is because the HLW glass (BSC 2004 [DIRS 167619], Section 8.1) degradation model has only a slight dependence on pH in the range of the deliquescence brines, and the DSNF degradation model (BSC 2003 [DIRS 163693], Section 8) has no pH dependence. Nevertheless, since no credit is taken for DSNF cladding, and sensitivity calculations indicate dose is not sensitive to degradation of HLW glasses (BSC 2003 [DIRS 168796], Sections 3.3.6 and 3.5) or release of DSNF (BSC 2003 [DIRS 163693], Section 6.4), preferential condensation due to colocation of waste is excluded based on low consequence.

The nature of flow through fractured, unsaturated host rock and a small, but sufficient, separation of neighboring waste packages mean that any chemical interactions between colocated waste packages would be unlikely and of negligible consequence. Unsaturated flow in the drift is largely vertical and colocated packages in the same disposal elevation would not interact geochemically. Hence, significant changes in the rates of waste package degradation and radionuclide mobilization due to chemical reactions between colocated waste packages are not

expected and chemical interactivity between colocated waste packages can therefore be excluded based on low consequence.

The possible effects of colocation with low- and intermediate-level radioactive waste, or toxic chemical wastes are moot. These waste types are not part of the license application design. In 10 CFR 63.73 [DIRS 156605], the NRC requires prompt notification if there are significant deviations from the design criteria and design bases stated in the license application. Any significant deviations with the potential to affect repository performance will be evaluated, and corrected, as needed. This ensures a low consequence (it is unlikely that there will be significant effects from "non-design" waste) in the event that the design is not followed. Therefore, the effects of colocation with other waste types are excluded based on low consequence.

### **TSPA Disposition:**

N/A

# **Supporting Documents:**

BSC 2003 [DIRS 163693]

#### **Related FEPs:**

- 2.1.01.01.0A, Waste inventory
- 2.1.01.02.0B, Interactions between codisposed waste
- 2.1.01.03.0A, Heterogeneity of waste inventory
- 2.1.02.01.0A, DSNF degradation (alteration, dissolution, and radionuclide release)
- 2.1.02.03.0A, HLW glass degradation (alteration, dissolution, and radionuclide release)

# **6.2.4** Interactions Between Codisposed Waste

#### **FEP Number:**

2.1.01.02.0B

**FEP Description**: Codisposal refers to the disposal of different waste types within the same waste package. Codisposal might affect chemical interactions or radionuclide mobilization. At Yucca Mountain, the DSNF will be combined with HLW canisters within a waste package. This codisposal with HLW within a waste package is unique to the DSNF and does not apply to the CSNF placement within waste packages.

The DSNF will be contained within canisters that will be placed within the waste packages. The use of canisters within the waste package is not typical of the CSNF placement within waste packages. Also, some DSNF waste packages may contain only DSNF canisters, while others may contain both DSNF and HLW canisters.

#### **Descriptor Phrases:**

Codisposed waste (chemical interactions between DSNF and HLW) Effects of HLW pour canisters Effects of DSNF high integrity canisters

#### **Screening Decision:**

Included

### **Screening Argument:**

N/A

TSPA Disposition: Codisposal issues include chemical interactions between the two degrading waste forms and the corroding HLW glass and DSNF canisters that occur through the solution chemistry within a breached waste package. The TSPA-LA will not take credit for the HLW glass pour canisters or the DSNF canisters or cladding as barriers to radionuclide release, but will account for the effects of container corrosion on the in-package chemistry. Different codisposal waste packages will have different amounts of DSNF and HLW glass, and thus different relative surface area accessible to water contact. The HLW glass release calculation depends on the surface area of glass contacted by water (BSC 2004 [DIRS 167619], Section 8.2.1), but the SNF degradation model assumes complete dissolution in one TSPA time step and is thus not sensitive to exposed surface area (CRWMS M&O 1998 [DIRS 100362], Tables 6-29 and A6-12). The geometric surface area used to represent all HLW glass in the HLW glass model (BSC 2004 [DIRS 167619], Section 8.2.1) is based on a weighted average of canister sizes. Neither the HLW glass degradation model nor the radionuclide inventory model distinguishes the contents of codisposal packages.

Codisposal waste packages are specially designed waste packages that will contain the HLW These packages are expected to be generally cooler glass and DSNF waste forms. (CRWMS M&O 1998 [DIRS 105649]; CRWMS M&O 2000 [DIRS 153595]) than CSNF packages. Current plans call for most codisposal waste packages to contain five glass logs and one DSNF canister (DOE 2002 [DIRS 158405], Section 9), but some codisposal waste packages will contain two HLW glass canisters, and one potential configuration will contain five (Hanford) HLW glass canisters with no DSNF (BSC 2003 [DIRS 161961], Table 17). The codisposal packages will be colocated randomly within an array comprised predominantly of CSNF waste packages, and will contain a relatively small fraction of the total waste. Interactions of condensed water or seepage with DSNF and HLW glass in a breached codisposal waste package were simulated in *In-Package Chemistry Abstraction* (BSC 2003 [DIRS 161962]), which uses degradation models for DSNF (BSC 2003 [DIRS 163693] and HLW glass (BSC 2004 [DIRS 167619]) with degradation models for other waste package components. Condensed and seepage water compositions are used to calculate the range of water chemistries (e.g., pH) that could occur in a breached codisposal waste package. Degradation of HLW glass tends to generate high pH solutions (BSC 2003 [DIRS 161962], Section 6.6.2), while DSNF degradation generates neutral pH solutions (BSC 2003 [DIRS 161962], Section 6.6.2). Those calculations indicate that the combined effects of degrading pour canisters, DSNF, and other waste package materials will moderate the pH values attained in condensed water and seepage water (BSC 2003 [DIRS 161962]).

The resulting in-package water chemistry is provided to TSPA-LA as part of *In-Package Chemistry Abstraction* (BSC 2003 [DIRS 161962]). The abstraction provides TSPA-LA parameters for the pH, Eh, ionic strength, and the total carbonate, chloride, and fluoride concentrations under condensed water and seepage conditions in a codisposal package. The DSNF release rate model has no explicit dependence on water chemistry effects and will not be affected by changes in the solution chemistry that occur due to chemical interactions between codisposal packages or between waste forms within a package (BSC 2003 [DIRS 163693]).

The glass degradation rate model does contain an explicit pH dependence and will be affected by changes in the solution pH within a codisposal package (BSC 2003 [DIRS 161962]. The glass model does not depend on other properties of the solution.

Thermal effects and preferential condensation due to codisposed waste are discussed as part of FEP 2.1.01.02.0A.

## **Supporting Documents:**

BSC 2003 [DIRS 161962] BSC 2003 [DIRS 163693] CRWMS M&O 1998 [DIRS 105649] CRWMS M&O 2000 [DIRS 153595] BSC 2004 [DIRS 167619]

#### **Related FEPs:**

2.1.01.02.0A

## **6.2.5** Heterogeneity of Waste Inventory

#### **FEP Number:**

2.1.01.03.0A

**FEP Description**: Commercial spent nuclear fuel (CSNF), DOE-owned spent nuclear fuel (DSNF), and high-level waste (HLW) shipped to the repository may contain quantities of radionuclides that vary from waste package to waste package, fuel assembly to fuel assembly, and from canister to canister. The composition of each of these waste forms may vary due to initial uranium enrichment, possible plutonium enrichment, and burnup of the fuel, among other factors. The physical state within the waste form may also vary. For example, damaged fuel pellets or extremely high-burnup fuels may have greater surface area exposed to any water penetrating a waste package than undamaged, low burnup spent fuel. Given these potential differences in isotopic composition and physical condition, the mass of radionuclides available for transport may vary significantly among waste packages.

The different physical (structure, geometry), chemical, and radiological properties of the many forms of CSNF, DSNF, and HLW could result in differences in the corrosion and alteration rates of the waste-package composition. This could affect repository chemistry, breach times, dissolution rates, and availability of radionuclides for transport.

## **Descriptor Phrases:**

Variation in radionuclide activity per waste package CSNF waste package configurations DSNF and HLW codisposed waste package configurations Spatial heterogeneity in-package (waste form, cladding, waste type)

#### **Screening Decision:**

Included

## **Screening Argument:**

N/A

TSPA Disposition: As discussed in Initial Radionuclide Inventories (DOE 2003 [DIRS 161961]) the repository waste types are quite heterogeneous in type (SNF versus glass) and in inventory per package. CSNF, DSNF, and HLW glass shipped to the repository will contain quantities of radionuclides that will vary from waste package to waste package, canister to canister, and fuel assembly to fuel assembly. The different physical, chemical, and radiological properties of the various CSNF, DSNF, and HLW glass waste forms could result in differences in their corrosion rates. This heterogeneity is represented in TSPA-LA by sampling from distributions for radionuclide inventory (for release calculations). However, for postclosure TSPA, the only simulations that approach the regulatory dose limit in 10,000 years are those where many packages breach. With many packages breached, the heterogeneity of the inventory, while included, is of minor importance and is characterized with the uncertainty parameters for the average CSNF, DSNF, and HLW glass radionuclide inventory in average CSNF and codisposal packages.

As discussed in *Defense HLW Glass Degradation Model* (BSC 2004 [DIRS 167619]), one effect of the heterogeneity of the waste inventory is variations in the compositions of waste glasses made to immobilize specific wastes at different DOE sites. The effect of waste glass compositions on the calculated degradation rate is taken into account through the range of values of the model parameter  $k_E$ . Ranges for the values of  $k_E$  in acidic and alkaline solutions are selected based on the results of laboratory tests with glasses that provide a wide range of compositions that bounds the range of concentrations of key glass components in HLW glasses, such as aluminum (BSC 2004 [DIRS 167619], Sections 6.5.4.2 and 6.5.2). The glass degradation model accounts for the heterogeneity of the waste inventory through the range of parameter values. The range of glass degradation rates calculated using the glass degradation model developed in *Defense HLW Glass Degradation Model* (BSC 2004 [DIRS 167619]) can be used with the average radionuclide concentrations for the entire HLW inventory.

## **Supporting Documents:**

BSC 2004 [DIRS 167619] BSC 2003 [DIRS 161961]

#### **Related FEPs:**

2.1.01.01.0A, Waste Inventory

## 6.2.6 DSNF Degradation (Alteration, Dissolution, and Radionuclide Release)

#### **FEP Number:**

2.1.02.01.0A

**FEP Description**: DSNF to be disposed of in Yucca Mountain has a variety of fuel types that include metallic uranium fuels; oxide and mixed oxide fuels; Three Mile Island rubble; and heterogeneous fuels such as UAlx, U-ZrHx, and graphite fuels. In general, the composition and structure of these spent nuclear fuels are significantly different from the commercial spent nuclear fuel (CSNF), and degradation, alteration, and dissolution may be different from the

CSNF degradation. Processes to be considered in this FEP include alteration and dissolution of the various DSNF waste forms, phase separation, oxidation of spent fuels, selective leaching, and the effects of the high-integrity can (HIC) on DSNF degradation.

## **Descriptor Phrases:**

DSNF inventory characteristics (surface area, fuel type)

Time-dependent THC characteristics in-package (temperature, pH, Eh, water concentration)

Degradation (corrosion/oxidation) of DSNF fuel matrix

Alteration of DSNF fuel matrix

Release from DSNF fuel matrix (congruent dissolution)

Release from DSNF fuel matrix (phase separation)

Release from DSNF fuel matrix (selective leaching)

Degradation (corrosion) of DSNF non-fuel metals

Release from DSNF (non-fuel metals)

N-Reactor uranium metal fuel

Pu ceramic waste

Naval fuel

Spatial heterogeneity of DSNF degradation

## **Screening Decision:**

Included

## **Screening Argument:**

N/A

**TSPA Disposition**: DSNF to be disposed of in Yucca Mountain is composed of a variety of fuel types that are not similar to the CSNF disposed waste. The various DSNF types have been classified into eleven groups for the purpose of TSPA-LA analyses (DOE 2000 [DIRS 118968]). Section 6.3 of *DSNF and Other Waste Form Degradation Abstraction* (BSC 2003 [DIRS 163693]) describes the development of upper-limit, conservative, and best estimate degradation models for each of 11 DSNF waste groups for TSPA-LA. These degradation models are summarized in Table 6 of *DSNF and Other Waste Form Degradation Abstraction* (BSC 2003 [DIRS 163693]).

The largest single DSNF type is the N-Reactor SNF, which comprises approximately 84 percent by weight of the total DSNF. When group-specific degradation models applicable to individual waste packages are not required, the N-Reactor SNF uranium metal (Group 7) models are adopted as a surrogate for all DSNF groups, except for the naval SNF (Group 1) (BSC 2003 [DIRS 163693]). The CSNF degradation model (BSC 2004 [DIRS 167321]) is used as the surrogate for naval SNF. For all groups (except naval DSNF), the upper-limit model produces complete dissolution of the waste form during a single code time step upon exposure of the waste form to groundwater (BSC 2003 [DIRS 163693], Section 7).

In addition to being the largest DSNF inventory type by weight, the N-Reactor SNF degradation models can be applied to the other DSNF groups (with the exception of Naval fuel) because a significant fraction of the N-Reactor SNF will be damaged at the time of emplacement in their

canisters and because the N-Reactor SNF degradation modelpredicts dissolution rates greater than most other groups. The two groups with potentially greater dissolution rates than N-Reactor SNF are mixed-carbide-fissile fuel waste particles in a nongraphite matrix (Group 3) and the immobilized ceramic Pu disposal waste form. Group 3 waste would not serve as an appropriate DSNF degradation surrogate because the total inventory of the Group 3 SNF is less than 0.001 percent of DSNF waste (DOE 2002 [DIRS 158405], Appendix D). For the immobilized ceramic Pu disposal waste form, the degradation model is either the instantaneous release of all the Pu from the waste package upon postclosure contact with groundwater, a ceramic dissolution rate, or ten times the ceramic dissolution rate. The models do not take credit for the glass-matrix coverage of surface areas on the Pu ceramic disks. Although the large majority of the excess defense plutonium was originally meant to be disposed in the repository as this "can-in-canister" form, the DOE Office of Environmental Management has recently decided to use the majority of the excess defense plutonium as MOX fuel in commercial reactors as the preferred disposition path rather than immobilization in a ceramic waste form (67 FR 19432 [DIRS 162618]).

Up to 50 percent of the DSNF cladding may be already perforated (Rechard 1995 [DIRS 101084], Section 11.3.1, p. 11-24). Because the cladding integrity of most DSNF will not be extensively characterized, the TSPA takes no credit for delayed degradation of the DSNF due to DSNF cladding or delayed release of radionuclide by the DSNF cladding (Section 5.2.6 of this analysis report). Also, the TSPA takes no credit for DSNF canister integrity (i.e., once the waste package has leaked or failed, it is conservatively assumed that the DSNF is directly exposed to the water or air of the repository environment).

An upper-limit degradation model is used for DSNF in TSPA-LA because preliminary analyses (Thornton 1998 [DIRS 125082]); Thornton 1998 [DIRS 107796]) have shown that overall repository performance is not sensitive to the DSNF degradation rate. This model yields complete dissolution of DSNF waste forms during a single code time-step upon exposure of the waste form to groundwater. The DSNF waste is a small percent of the total waste to be disposed and the waste stream plume is dominated by CSNF degradation even when upper-limit DSNF degradation models are used. The formulation of the conservative and best-estimate models is described in *DSNF and Other Waste Form Degradation Abstraction* (BSC 2003 [DIRS 163693], Section 6.2.7).

#### **Supporting Documents:**

BSC 2003 [DIRS 163693]

#### **Related FEPs:**

- 2.1.01.02.0A, Interactions between colocated waste
- 2.1.01.02.0B, Interactions between codisposed waste

## 6.2.7 CSNF Degradation (Alteration, Dissolution, and Radionuclide Release)

#### **FEP Number:**

2.1.02.02.0A

**FEP Description**: Alteration of the original mineralogy of the commercial spent nuclear fuel (CSNF) (under wet or dry conditions) and dissolution of the uranium-oxide matrix can influence

the mobilization of radionuclides. The degradation of UO<sub>2</sub> could be affected by a number of variables, such as surface area, burnup, temperature, overall solution electrochemical potential (Eh), pH, and especially solutions containing significant concentrations of calcium, sodium, carbonate and silicate ions, as well as availability of organic complexing materials. In turn, these water properties are affected by the alteration of the cladding and matrix.

# **Descriptor Phrases:**

CSNF inventory characteristics (surface area, burnup)

Time-dependent THC characteristics in-package (temperature, pH, Eh, water concentration)

Degradation of CSNF uranium oxide fuel matrix

Alteration of CSNF uranium oxide fuel matrix

Release from CSNF fuel matrix (congruent dissolution)

Release from CSNF fuel matrix (phase change)

Release from CSNF fuel matrix (selective leaching)

Degradation (corrosion) of CSNF nonfuel metals

Release from CSNF (nonfuel metals)

Spatial heterogeneity of CSNF degradation

# **Screening Decision:**

Included

## **Screening Argument:**

N/A

**TSPA Disposition**: As described in CSNF Waste Form Degradation: Summary Abstraction (BSC 2004 [DIRS 167321]), the base case CSNF model is designed to provide the fractional release rate of radionuclides (F<sub>i</sub>) when the CSNF matrix is dissolved or otherwise altered upon exposure to water or humid air. The CSNF alteration and dissolution processes that are considered are described in Section 6.2 of CSNF Waste Form Degradation: Summary Abstraction (BSC 2004 [DIRS 167321]). The mathematical form of the model is described in Section 1 of CSNF Waste Form Degradation: Summary Abstraction (BSC 2004 [DIRS 167321]). It has six model parameters (A, a<sub>0</sub>, a<sub>1</sub>, a<sub>2</sub>, a<sub>3</sub> and a<sub>4</sub>) and four independent variables (absolute temperature, pCO3, pO2, and pH). The effects of surface area are included through the effective specific surface area parameter (A) as described in CSNF Waste Form Degradation: Summary Abstraction (BSC 2004 [DIRS 167321], Section 6.4.1.5). Effects of other factors, including burnup, secondary phase formation, and selective or congruent release, are discussed in CSNF Waste Form Degradation: Summary Abstraction (BSC 2004 [DIRS 167321], Section 6.2.2.3). The determination of the model parameter values over the independent variables factor space of interest is described in CSNF Waste Form Degradation: Summary Abstraction (BSC 2004 [DIRS 167321], Section 6.4.1).

In TSPA-LA, the CSNF degradation model parameters are used along with the in-package chemistry to calculate a CSNF degradation rate at each model time step. The degradation model parameters are determined by sampling from parameter distributions that incorporate uncertainty, while the in-package chemistry variables are calculated as part of the TSPA simulation.

## **Supporting Documents:**

BSC 2004 [DIRS 167321]

#### **Related FEPs:**

- 2.1.01.02.0A, Interactions between colocated waste
- 2.1.01.02.0B, Interactions between codisposed waste

## 6.2.8 HLW Glass Degradation (Alteration, Dissolution, and Radionuclide Release)

#### **FEP Number:**

2.1.02.03.0A

**FEP Description**: Glass waste forms are thermodynamically unstable over long time periods and will alter on contact with water. Radionuclides can be mobilized from the glass waste by a variety of processes, including degradation and alteration of the glass, phase separation, congruent dissolution, precipitation of silicates, coprecipitation of other minerals including iron corrosion products, and selective leaching.

## **Descriptor Phrases:**

HLW glass inventory characteristics (surface area, composition)

Time-dependent THC characteristics in-package (temperature, pH, water concentration)

Degradation (corrosion) of HLW glass

Alteration of HLW glass

Release from HLW glass (congruent dissolution)

Release from HLW glass (phase separation)

Release from HLW glass (selective leaching)

Release from HLW glass (precipitation of silicates and other minerals)

Spatial heterogeneity of HLW glass degradation

#### **Screening Decision:**

Included

## **Screening Argument:**

N/A

**TSPA Disposition**: The rate expression for glass degradation provided in *Defense HLW Glass Degradation Model* (BSC 2004 [DIRS 167619]) was developed to address this FEP. The model addresses degradation of glass exposed to humid air or dripping water, and glass immersed in water. The glass degradation rate is calculated as a function of pH and temperature by using the following equation: rate  $G = k_E 10^{(npH)}$  exp<sup>(-Ea/RT)</sup> (BSC 2004 [DIRS 167619], Section 6.5.2 and Equation 9). This rate accounts for the combined effects of water diffusion, ion exchange, and hydrolysis processes that lead to glass degradation when contacted by water. Explicit dependencies are given for variables tracked in TSPA calculations, including pH, temperature, and relative humidity (rate G is defined as zero for relative humidities less than 44 percent). The effects of environmental processes specific to the disposal conditions that affect glass degradation, such as water condensation and dripping, are captured in the model by the range of values of the  $k_E$  term. The results of tests in which those processes occur are used to determine bounding model parameter values. The range of  $k_E$  also accounts for the range of glass

durabilities (compositions) and the evolution of the solution chemistry contacting the glass. Although the rate equation does not depend on time, variables used in the model–pH, temperature, and relative humidity–depend on time; therefore, those values must be obtained from other models. The release of radionuclides from HLW glass is modeled to be congruent with other glass matrix components. The release rates of boron measured in laboratory tests are used to determine the matrix degradation rate. The radionuclide release rate is calculated as the product of the glass degradation rate, the exposed surface area, and the radionuclide inventory. The model report (BSC 2004 [DIRS 167619]) provides equations for calculating the glass degradation rate and the surface area; the radionuclide inventory is provided by another model.

Surrogate glasses having glass matrix compositions representative of HLW glasses were used in laboratory tests. Except for the absence of radionuclides, these glasses provided levels of glass and glass phase separation and devitrification phases representative of HLW glasses. The maximum rates calculated by the model were selected to bound the rates measured experimentally after the precipitation of silicate, iron silicate, and mineral phases. In this way, processes that affect the glass alteration rate, congruent dissolution, selective leaching, and precipitation of alteration phases, have been implicitly incorporated in the model through model parameters, even though only the temperature and pH dependencies are calculated explicitly. The range of values of the rate coefficient  $k_{\rm E}$  provides rates consistent with those measured under various test conditions in which glasses were reacted in humid air, dripping water, and various immersion conditions. A triangular distribution of values for  $k_{\rm E}$  is skewed to low values to reflect the greater likelihood that glass in the disposal system will be contacted by water vapor (which gives the lowest measured rates) rather than immersion (which gives the highest measured rates). A minimum relative humidity of 44 percent is required for glass degradation to occur (BSC 2004 [DIRS 167619], Section 6.5.5.3.2).

The range of  $k_E$  also reflects the effects of glass composition and, to a large extent, the radionuclide inventory on glass degradation, since the waste glasses are formulated based on the waste compositions. Calculation of the radionuclide release rate accounts for the spatial heterogeneity of HLW glass (i.e., the distribution of various HLW glass) by using a representative glass log to represent all HLW glasses. The mass and surface area of glass that is available for corrosion, and the average radionuclide inventory, are calculated based on the characteristics and predicted numbers of glass logs to be received from different production facilities.

In TSPA-LA, the HLW degradation model parameters and factors are used along with the in-package chemistry to calculate a HLW degradation rate at each model time step. The degradation model parameters and factors are determined by sampling from parameter distributions that incorporate uncertainty, while the in-package chemistry parameters are calculated as part of the TSPA simulation. The composition of the representative glass is not defined in the HLW glass degradation model or used to calculate the degradation rate. A representative composition is specified in the in-package chemistry model for calculating the effects of glass dissolution on the chemistry.

## **Supporting Documents:**

BSC 2004 [DIRS 167619]

#### **Related FEPs:**

2.1.01.02.0A, Interactions Between Colocated Waste 2.1.01.02.0B, Interactions Between Codisposed Waste

# 6.2.9 Alpha Recoil Enhances Dissolution

#### **FEP Number:**

2.1.02.04.0A

**FEP Description**: During decay of certain radionuclides, alpha particles may be emitted with sufficiently high energies that the daughter nuclide recoils appreciably to conserve system momentum. A potential result of recoil is that certain radionuclides, such as <sup>234</sup>U, exhibit substantially greater dissolution rates (with the same solubility limits) and can be transported preferentially.

## **Descriptor Phrases:**

Alpha decay recoil enhances waste dissolution

## **Screening Decision:**

Excluded (low consequence)

Screening Argument: The effects of alpha recoil can be excluded based on low consequence. Omission of the effects of alpha recoil will not significantly change radionuclide releases to the accessible environment, because the alpha recoil enhanced dissolution rates have been shown to be much less than the dissolution rate due to chemical processes. Even when conservatively assuming that all radioactive decay results in alpha recoil, it does not cause significant increases in the dissolution rate of the different waste forms. The processes investigated in this argument only involve direct nuclear effects, and not indirect nonnuclear effects such as thermal-enhanced dissolution due to heat generation from the radioactive decay of SNF. The following is the detailed discussion.

Of the various radioactive decay modes (i.e., alpha ( $\alpha$ ), beta ( $\beta$ ), gamma ( $\gamma$ ), spontaneous fission [SF], isomeric transition, etc.) the most important for fissile materials is the alpha decay mechanism. This mechanism is the dominant decay mode for heavy radionuclides. All the heavy nuclides above 209Bi are radioactive and tend to decay into more stable nucleus configurations (i.e., atomic masses of less than 200 atomic mass units). Because these heavy radionuclides need to lose significant quantities of mass in order to become more stable, in general they will decay by the mode that results in the largest mass loss. Thus, the most likely decay mode will be alpha decay, which has the largest mass and associated kinetic energy. Although many of the heavy radionuclides emit alpha particles with energies greater than 4.0 MeV (Parrington et al. 1996 [DIRS 103896], p. 48), there is no gamma decay or beta decay with energy greater than 4.0 MeV and only a few with energy greater than 1.0 MeV. Thus, alpha recoil mechanisms will bound the effects due to beta and gamma recoil. Other special decay modes such as isomeric transition and spontaneous fission decay have probabilities of occurrence that are orders of magnitude less than that of alpha decay. Information in Attachment II of this analysis report indicates that isomeric transition occurs for <sup>108m</sup>Ag, <sup>242m</sup>Am, <sup>93m</sup>Nb, and <sup>121m</sup>Sn; none of which are significant in terms of mass contribution. Also, information from Lederer and

Shirley (1978 [DIRS 142133], p. 1464) indicates that the spontaneous fission half-lives are several orders of magnitude longer than that for other decay modes and are, thus, insignificant.

The number of atom displacements per alpha decay can be calculated by noting that when a recoil nucleus strikes an atom, it requires a minimum displacement energy,  $E_d$ , of approximately 25 eV to eject the struck atom from its lattice site (Foster and Wright 1973 [DIRS 144061], p. 296). The total number of displacements caused by a single alpha decay event is given by Equation 1 (Foster and Wright 1973 [DIRS 144061], p. 296). Equation 1 gives displacement units:

$$Disp(E) = \int_{0}^{\infty} P(T)K(E,T)v(T)dT = \int_{E_{d}}^{T_{m}} P(T)K(E,T)v(T)dT$$
 (Eq. 1)

where

P(T) = probability that an atom (primary knock-on), struck by either the emitted alpha or the alpha recoil atom, receiving energy T is displaced.

K(E,T) = probability for the transfer of kinetic energy T to the primary knock-on atom of energy E.

v(T) = total number of displacements in a cascade originating from a primary knockon atom whose energy is T.

The expression is integrated over the energy range starting at the displacement threshold energy,  $E_d$ , and ending at the maximum energy that can be transferred to an atom,  $T_m$ . Since the displacement of atoms corresponds to a threshold event, P(T) is modeled as a Heaviside step function (Foster and Wright 1973 [DIRS 144061], p. 297):

$$P(T) = \langle T - E_d \rangle^0 = \begin{cases} 0 & \text{if } T < E_d \\ 1 & \text{if } T \ge E_d \end{cases}$$
 (Eq. 2)

To simplify the analysis, the probability for kinetic energy transfer is treated as being a uniform distribution over the applicable energy range:

$$K(E,T) = \frac{1}{T_m - E_d}$$
 (Eq. 3)

The total number of displacements which originate from a primary knock-on is described by the Kinchin-Pease Model (Foster and Wright 1973 [DIRS 144061], p. 297):

$$\nu(T) = \frac{T}{2E_d} + \frac{E_i - T}{2E_d} \langle T - E_i \rangle^0 = \begin{cases} T / 2E_d & \text{if } T \le E_i \\ E_i / 2E_d & \text{if } T > E_i \end{cases}$$
 (Eq. 4)

where

 $E_i$  = energy required for ionization.

The  $2E_d$  in the denominator accounts for the displacement of the knock-on atom and the additional  $E_d$  for the striking atom to also leave the displacement site. The model also

reasonably concludes there is an ionization threshold ( $E_I \approx 1000A$ ) below which displacements take place and above which only ionization takes place.

The total number of displacements is given by Equation 5, which includes ionization interactions.

$$Disp(t_{m}) = \begin{cases} \int_{E_{d}}^{T_{m}} \frac{T}{2E_{d}T_{m} - 2E_{d}^{2}} dT & \text{if } T_{m} \leq E_{i} \\ \int_{E_{d}}^{E_{i}} \frac{T}{2E_{d}T_{m} - 2E_{d}^{2}} dT + \int_{E_{i}}^{T_{m}} \frac{E_{d}}{2E_{d}T_{m} - 2E_{d}^{2}} dT & \text{if } T > E_{i} \end{cases}$$

$$= \begin{cases} \frac{T_{m} + E_{d}}{4E_{d}} & \text{if } T_{m} \leq E_{i} \\ \frac{E_{i}^{2} - E_{d}^{2}}{4E_{d}(T_{m} - E_{d})} + \frac{E_{i}T_{m} - E_{i}^{2}}{2E_{d}(T_{m} - E_{d})} & \text{if } T_{m} > E_{i} \end{cases}$$
(Eq. 5)

For the example involving  $^{238}$ U decaying to  $^{234}$ Th, there are two cases to examine. The first is for the alpha recoil atom, and the second is for the emitted alpha particles. From the analysis in Attachment III of this analysis report, it can be seen that the alpha recoil atom ( $^{234}$ Th) has a value 0.072 MeV for  $T_m$ , which is much less than the ionization energy (typically approximately 1000A equal to 0.234 MeV (million electron volts). This results in  $Disp_{max}(\alpha)$  equal to 720 displacements per alpha decay. (This does not include replacement collisions along with focusing and channeling effects, which will significantly lower the estimate for displacements.) If each of the secondary displacements follows a bifurcation process (i.e.,  $2^N$  equals 720), this would correspond to 9.49 bifurcation levels. This means that the maximum number of atom monolayers of the SNF fuel meat through which recoil nuclei (due to alpha decay) could pass through and enter bounding groundwater is approximately 10. This is only for recoil atoms traveling in the direction of the groundwater. Attachment III of this analysis report indicates that only half of the recoil could be in the proper direction. This also does not mean that all the (secondary) displaced atoms within ten monolayers of the material surface would enter the groundwater; it only indicates that it is possible.

The second case, the emitted alpha particles, involves a much larger number of possible displacements. This is due to its larger kinetic energy. From Lederer and Shirley (1978 [DIRS 142133]), it can be identified that the maximum energy for alpha particles emitted from  $^{238}$ U is 4.196 MeV. Since this energy is above the ionization value, the second version of Equation 5 that contains two terms must be used to take into account the ionization by the alpha particles. Using the maximum alpha energy results in a value of 4,550 for  $Disp(\alpha)$ . When added to the recoil atom value, the net displacements are 5,270, which corresponds to approximately 12.4 bifurcation levels.

The enhancement to the dissolution rate due to alpha decay can now be upper bounded. This rate will correspond to the number of alpha decays per unit time within the first thirteen half-monolayers of the material surface that result in nuclei recoiling toward the groundwater. The worst case density for thorium (or even uranium) will be approximately that of pure plutonium metal, with a maximum density of 19.84 g/cm<sup>3</sup> (Wick 1980 [DIRS 143651], Table 7.1) and a

monolayer thickness of approximately 3.0 Å (3.0x10<sup>-10</sup>m). The combination of these two parameters results in 0.039 grams of SNF material within the first thirteen monolayers of a surface area of 1.0 m<sup>2</sup> that are in the direction of the material surface. When this surface density (0.039 g/m<sup>2</sup>) is multiplied by the fractional rate at which the SNF material experiences radioactive α-decay, it can be expressed in the units used in the CSNF (BSC 2004 [DIRS 167321]; DSNF (BSC 2003 [DIRS 163693]) degradation analysis reports for dissolution of both CSNF and DSNF material due to chemical processes. The fractional rate was determined from radiological half-lives along with some data from Attachment II of this analysis report, which contains inventory information for the Yucca Mountain repository. These data identify the major constituents on a mass basis of the final waste forms (SNF and HLW): <sup>238</sup>U, <sup>235</sup>U, <sup>239</sup>Pu, <sup>236</sup>U, and <sup>240</sup>Pu. Key radionuclides from Attachment II of this analysis report are analyzed in Table 6.2-1, which identifies their maximum alpha recoil enhancement for dissolution rates. Data in column 5 of this table are computed by noting that the fractional decay rate for the radionuclides is given by their decay constant ( $\lambda = ln(2)/\tau_{1/2}$ ). To put these values from Table 6.2-1 into proper perspective, a comparison to Figure 2 must be made. Figure 2 identifies the dissolution rates of different waste forms due to chemical (nonnuclear) processes. As can be identified, the alpha recoil dissolution rates are much less than the values due to chemical processes.

In summary, the radioactive decay processes that directly increase fuel-meat dissolution are bounded by alpha recoil rates. Even when conservatively assuming that all radioactive decays result in an alpha recoil, they will not cause significant increases to the dissolution rate of the different waste forms. The processes investigated in this argument are only for direct nuclear effects and not indirect nonnuclear effects, such as thermally enhanced dissolution due to heat generation from SNF radioactive decay. Thus, the overall dissolution due to direct nuclear decay processes has been eliminated from performance-assessment calculations on the basis of low consequence.

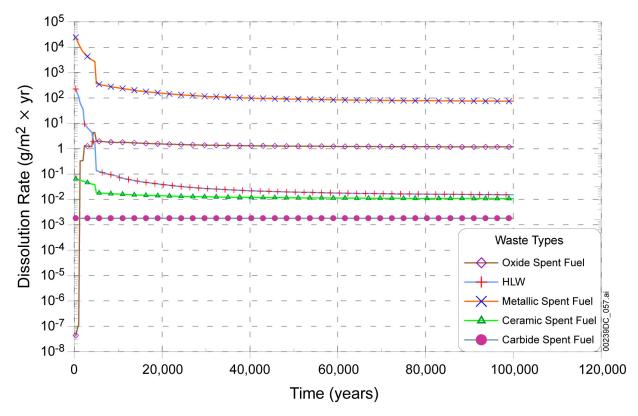
Table 6.2-1. Alpha Recoil Enhanced (From  $\alpha$  and  $\alpha$ -Recoil Atom) Dissolution Rates Due to the Major Mass-Based Constituents of SNF and HLW to be Disposed of in the Yucca Mountain Repository

Nuclide ID	Decay Mode	Half–Life <sup>(a)</sup> (years)	Fraction Decay Rate <sup>(b)</sup> (1/yr)	α–Decay Rate in 13 Mono-Layers <sup>(c)</sup> (g/m²–yr)
<sup>238</sup> U	α, γ, SF	4.47 x 10 <sup>9</sup>	1.55 x 10 <sup>-10</sup>	6.05 x 10 <sup>-12</sup>
<sup>235</sup> U	α, γ, SF	7.04 x 10 <sup>8</sup>	9.85 x 10 <sup>-10</sup>	3.84 x 10 <sup>-11</sup>
<sup>239</sup> Pu	α, γ, SF	2.410 x 10 <sup>4</sup>	2.88 x 10 <sup>-5</sup>	1.12 x 10 <sup>-6</sup>
<sup>236</sup> U	α, γ, SF	2.342 x 10 <sup>7</sup>	2.96 x 10 <sup>-8</sup>	1.15 x 10 <sup>-9</sup>

NOTES: <sup>a</sup> Data obtained from Attachment II of this analysis report. The original source of information, in radioactivity units, was DOE (1998 [DIRS 122980]). Mass unit values were derived by Sanchez et al. (1998 [DIRS 149368]).

<sup>&</sup>lt;sup>b</sup> The fraction decay rate, also known as the decay constant, is given by  $\lambda = \ln(2)/\iota \frac{1}{2}$ , where  $\iota \frac{1}{2}$  is the radionuclide half-life given by values in column 3.

<sup>&</sup>lt;sup>c</sup> Each monolayer thickness is 3.0 Å (3.0x10-10m), and the density is upper bounded at 19.86 g/cm3 (theoretical density of pure plutonium metal ([Wick 1980 [DIRS 143651]).



Source: CRWMS M&O 1998 [DIRS 100362], p. A6-29, Figure A6-1

Figure 2. Comparison of Dissolution Rates for High-Level Radioactive Waste, Metallic Carbide, and Ceramic Spent Nuclear Fuel

# **TSPA Disposition:**

N/A

## **Supporting Documents:**

None.

## **Related FEPs:**

None.

## 6.2.10 HLW Glass Cracking

#### **FEP Number:**

2.1.02.05.0A

**FEP Description**: Cracking of the HLW glass on cooling and during handling means that the surface area of the glass is greater than the surface area of a monolithic block. The increase in the surface area could affect the rate of glass alteration and radionuclide dissolution.

## **Descriptor Phrases:**

Increased dissolution surface area from HLW glass cracking

## **Screening Decision:**

Included

## **Screening Argument:**

N/A

**TSPA Disposition**: The expression for exposed glass surface area developed to address this FEP is provided in *Defense HLW Glass Degradation Model* (BSC 2004 [DIRS 167619]). The surface area used to calculate the radionuclide release rate bounds the effects of thermal cracking during manufacture and impact cracking during subsequent handling. The exposure factor ( $f_{exposure}$ ) is used to model the combined effects of the added surface area due to cracking, the fraction of the surface that is accessible to water, and the reactivity of glass in tight cracks relative to glass at a free surface. The value of  $f_{exposure}$  is selected for each realization from a triangular distribution with a minimum and most expected value of 4 and a maximum value of 17. The initial exposed surface area is calculated by using the following equation (BSC 2004 [DIRS 167619], Section 6.5.6, Equation 37):

$$S_0 = f_{\text{exposure}} \times (2\pi r_0^2 + 2\pi r_0 \times L_0)$$
 (Eq. 6)

where  $r_0$  is the internal radius of the glass canister, and  $L_0$  is the length of the glass canister.

The change in the surface area as the glass degrades is calculated as the sum of the product of the specific surface area of a glass log and the mass of glass available at the beginning of the time step using the following equation (BSC 2004 [DIRS 167619], Section 6.5.6, Equation 39):

$$S = fexposure \times 2.70 \times 10-3 \text{ m2/kg} \times (2,710 \text{ kg} - \Sigma Mt \text{ kg})$$
 (Eq. 7)

where  $\Sigma M$  gives the mass loss during all previous time steps (and resulting loss of surface area).

The value of  $\Sigma M$  is calculated as the product of the glass degradation rate used for that time step and duration. The mass loss is used to calculate the loss in surface area.

# **Supporting Documents:**

BSC 2004 [DIRS 167619]

#### **Related FEPs:**

None

## 6.2.11 HLW Glass Recrystallization

#### **FEP Number:**

2.1.02.06.0A

**FEP Description**: HLW glass recrystallization could occur and would lead to a less corrosion-resistant waste form. Recrystallization is a slow process and typically occurs only if a high glass temperature is maintained over a prolonged period.

## **Descriptor Phrases:**

Increased corrosion from HLW glass crystallization

# **Screening Decision:**

Included

# **Screening Argument:**

N/A

**TSPA Disposition**: The effect of crystallization on the glass corrosion rate is implicitly accounted for in *Defense HLW Glass Degradation Model* (BSC 2004 [DIRS 167619]) by the range of model parameter values used to represent uncertainty. The ranges of model parameter values were determined from experimentally measured dissolution rates of glasses having compositions similar to HLW glasses.

Although the effects of crystallization are included in the TSPA-LA model, in situ devitrification of HLW glass is not expected to occur at disposal temperatures (i.e., at temperatures less than 400°C). As part of model validation, the glass degradation rate was shown to be insensitive to the presence of crystalline phases that are either formed by devitrification of the glass melt during manufacture or intentionally added to the waste form. This is based on literature results that show the effects of devitrification on glass dissolution rate are small and near the uncertainty in the measurement of the rate.

In summary, even though the effects recrystallization on the glass degradation rate are expected to be insignificant, the effects are captured in TSPA-LA through the range of parameter values used in the degradation model used to represent uncertainty.

# **Supporting Documents:**

BSC 2004 [DIRS 167619]

#### **Related FEPs:**

None.

# 6.2.12 Radionuclide Release from Gap and Grain Boundaries

#### **FEP Number:**

2.1.02.07.0A

**FEP Description**: While in the reactor at the high temperatures, radionuclides such as I and Cs may migrate and preferentially accumulate in cracks in the fuel matrix, grain boundaries of the UO<sub>2</sub>, and in the gap between the fuel and cladding. After the waste package fails and the cladding perforates, the release rate of this fraction of the radionuclides could be rapid. In addition, reactions between materials within the spent nuclear fuel assembly or waste package infill such as I and Pb may affect this process.

## **Descriptor Phrases:**

Rapid release from fuel gap and grain boundaries Chemical binding of gap inventory Migration to gap and grain boundaries after emplacement

## **Screening Decision:**

Included

## **Screening Argument:**

N/A

**TSPA Disposition**: Gap-and-grain boundary release applies mainly to commercial spent nuclear fuel and similar fuel designs (such as MOX) based on UO<sub>2</sub>-based fuel pellets. In such SNF a portion of some of the volatile or soluble fission product radionuclides can migrate to the fuel pellet grain boundaries and open gap areas of the fuel rods under the influence of the high temperature gradients operative under reactor operation. Further migration under the significantly cooler environment of repository disposal is not expected to occur. The gap-and-grain-boundary inventory is assumed in the TSPA to be accessible for dissolution into any water that penetrates the fuel cladding.

As described in *CSNF Waste Form Degradation: Summary Abstraction* (BSC 2004 [DIRS 167321]), the release of the gap and grain boundary radionuclide inventory is modeled as an instantaneous release fraction (f<sub>i</sub>) where the subscript i refers to <sup>137</sup>Cs, <sup>129</sup>I, <sup>90</sup>Sr, and <sup>99</sup>Tc. Available experimental data are used to estimate the mean values, the ranges and the distribution functions for f<sub>i</sub> (BSC 2004 [DIRS 167321], Section 6.3). The gap and grain boundary release is modeled as an instantaneous release in one GoldSim time step. These distributions are sampled at the beginning of each TSPA GoldSim realization to determine the values of f<sub>i</sub> that are used for the instantaneous release fractions when fuel cladding fails during the course of the realization. At the high temperatures fuel pellets experience during reactor operation, a significant migration of gaseous or soluble radionulides to the gap and grain boundaries occurs. At the much lower temperatures expected after waste package emplacement, the thermally driven migration of radionuclides to the gap and grain boundaries is expected to be low enough that it can be considered to be included in the uncertainties in the instantaneous release fraction of the CSNF (BSC 2004 [DIRS 167321], Section 6.2.1.2).

## **Supporting Documents:**

BSC 2004 [DIRS 167321]

#### **Related FEPs:**

2.1.02.02.0A, CSNF Degradation (Alteration, Dissolution, and Radionuclide Release)

# **6.2.13** Pyrophoricity from DSNF

#### **FEP Number:**

2.1.02.08.0A

**FEP Description**: DSNF can contain pyrophoric material. Pyrophoric material could ignite and produce an adverse effect on repository performance. Pyrophoric events could affect the thermal

behavior of the system and could contribute to degradation of the waste package, waste form, and cladding.

# **Descriptor Phrases:**

Effects of pyrophoricity (heat generation)
Effects of pyrophoricity (waste package degradation)
Effects of pyrophoricity (waste form degradation)
Effects of pyrophoricity (cladding degradation)

## **Screening Decision:**

Excluded –low consequence

Screening Argument: DSNF may potentially include pyrophoric material, particularly the N-Reactor SNF currently being removed from the K-basin and placed in dry storage at Hanford. Because N-Reactor SNF is composed primarily of zirconium-clad metallic uranium, it must be assessed for its potential for pyrophoric behavior. However, a significant amount of the cladding has been breached exposing metallic uranium, which has shown pyrophoric behavior in the past (Thornton 1998 [DIRS 125082]). Pyrophoric materials can spontaneously ignite and produce an adverse effect on repository performance by producing heat and dispersible particulates and gases. For the purposes of this analysis, pyrophoricity is understood to be the capability to ignite spontaneously if the temperature, chemical, or physical or mechanical conditions of the storage or transportation environments are oxidizing (ASTM C 1454-00 [DIRS 152779], Section 3.2), which could occur as a result of waste package degradation, mechanical impact, or overheating during handling or transportation. A pyrophoric event is defined as ignition, followed by rapid chemical oxidation or self-sustained burning. A pyrophoric event has the potential for increasing the release and dispersal rate of radionuclides, which could impact repository performance.

Uranium hydride inclusions in the metallic uranium matrix of damaged N-Reactor SNF (i.e., fuel elements that have damaged cladding) could provide an ignition source. The open literature contains descriptions of pyrophoric behavior in uranium metal and uranium metal-based SNF (such as Magnox SNF). Although N-Reactor SNF has significant damaged cladding and is known to contain such uranium hydride inclusions, there have not been any pyrophoric reactions during normal handling and testing of N-Reactor SNF samples at the K-basins or Pacific Northwest National Laboratory in support of the N-Reactor fuel interim dry storage program. However, N-Reactor SNF has displayed unexpected pyrophoric behavior during handling and processing in the air or water environments and aggressive mechanical handling conditions associated with reprocessing operations at Hanford and West Valley (Schulz 1972 [DIRS 159406]).

Since uranium hydride inclusions tend to be concentrated near the exposed uranium metal fuel surface of damaged SNF (Abrefah et al. 1999 [DIRS 151226]; Marschman et al. 1997 [DIRS 149429]), a small but finite chance of spontaneous ignition will be considered in this analysis to support the screening argument of low consequence of pyrophoric event to the postclosure TSPA-LA. Because the fraction of N-Reactor SNF with cladding that is damaged enough to expose the metallic uranium core is quantitatively unknown but potentially significant (Abrefah et al. 1995 [DIRS 151125]), all the SNF elements will be regarded as damaged for the purposes of this analysis.

If spontaneous ignition of U-hydrides occurs, there must be sufficient oxygen to support continuing combustion. This is unlikely, since waste packages containing potentially pyrophoric material will be filled with an inert gas prior to emplacement in the repository. Furthermore, the N-Reactor SNF will be contained within canisters (known as multicanister overpacks) emplaced inside the waste packages that are also filled with an inert gas. The inert environment will exclude all but small quantities of water and oxygen, thus reducing the potential for oxidation reactions prior to breach of the waste package (DOE 1998 [DIRS 122980], Section 5.1.2.1). If breach of the waste package and multicanister overpack occurs, the breach would be expected to be small enough that oxygen would leak slowly into the waste package. The slow introduction of oxygen would tend to limit the oxidation rate of any remaining hydrides, thus limiting the ability of the hydrides to initiate a pyrophoric event. However, there is not sufficient data available at this time to absolutely exclude pyrophoric events based on their low probability of occurrence. Therefore, the exclusion of this FEP from TSPA-LA is based on the fact that the potential adverse effects of a pyrophoric event , are insignificant.

Attachment I of this analysis report provides a consequence-based analysis that estimates the impact a pyrophoric event would have on repository performance. The analysis conservatively (but non-mechanistically) assumes that all N-Reactor SNF-containing waste packages that breach during the regulatory period undergo a pyrophoric event within one TSPA time step. It is also assumed that (1) breach of an N-Reactor SNF-containing waste package results in a pyrophoric condition that causes the two adjacent waste packages to fail, (2) the various types of waste packages are evenly distributed throughout the repository, and (3) the probability of failure of a waste package containing pyrophoric (i.e., N-Reactor) SNF is the same as that of any other waste package (Section 5.2.13 of this analysis report). The analysis demonstrates that a pyrophoric event involving waste packages containing N-Reactor SNF would not have a significant impact on postclosure repository performance in terms of impact on radionuclide release and peak offsite dose. This is primarily due to the fact that only a small fraction of the emplaced waste packages will contain N-Reactor SNF. In terms of the potential increase in total radionuclides released over the repository's lifetime, the impact of pyrophoric events would not exceed about a one percent increase in the total amount of radionuclides released. In terms of the peak offsite dose that could result from a single pyrophoric event, a pyrophoric event would, at most, cause a few percent increase in peak offsite dose above the dose that would be obtained if pyrophoric events were not possible. As for clustered events, unrealistic scenarios involving noncredible mechanisms would be required to generate more than a few percent increase in peak offsite dose. Therefore, pyrophoricity of DSNF can be excluded from further consideration based on low consequence to radiological exposures and radionuclide releases.

# **TSPA Disposition:**

N/A

# **Supporting Documents:**

N/A

#### **Related FEPs:**

- 2.1.11.01.0A, Heat generation in EBS
- 2.1.12.29.0A, Flammable Gas Generation from DSNF

## 6.2.14 Chemical Effects of Void Space in Waste Package

#### **FEP Number:**

2.1.02.09.0A

**FEP Description**: If waste packages and/or DSNF canisters are not completely filled, then the unfilled inert-gas or air-filled volume could influence water-chemistry calculations.

## **Descriptor Phrases:**

Chemical effects of void space in waste package

## **Screening Decision:**

Included

# **Screening Argument:**

N/A

**TSPA Disposition**: The base-case conceptual model for in-package chemistry is composed of two conceptual models, the no-drip model and the seepage dripping model, which are collectively referred to as the In-Package Chemistry Model (IPCM) in *In-Package Chemistry Abstraction* (BSC 2003 [DIRS 161962]). The water vapor condensation model addresses the situation in which water vapor enters the breached waste package and condenses. The seepage model addresses the situation in which liquid water seeps or drips into the breached waste package. These models differ from each other basically in the chemistry of the water to which the waste forms in a breached waste package are exposed. In evaluating the in-package water chemistry, the entire void volume in the waste package is taken to be saturated with liquid and gas and includes any void volume in a canister and any time-varying void volume in the waste form. The IPCM accounts for the unfilled void space in the waste package, and, thus, its impact on the in-package chemistry.

The conceptual model is an unsaturated model in which the void spaces within a waste package are partially filled by liquid water in equilibrium with atmospheric gases. Void space in the waste package is thus partially gas filled. This has the effect of putting the gas phase in close contact with the liquid- and solid-phase reactants in the system, and is in fact the basis of the conceptual model implemented in *In-Package Chemistry Abstraction* (BSC 2003 [DIRS 161962]). Thus, the increased void space in the waste package decreases the distance that gas must diffuse to maintain equilibrium with the liquid phase; this is contrast to the "bathtub" model (BSC 2003 [DIRS 161962], Section 6.3.1) where all of the void space is liquid-filled and the gas phase must diffuse much longer distances to maintain equilibrium.

The effects of the unfilled void space on the in-package chemistry are passed to TSPA explicitly via the oxygen and carbon dioxide equilibrium within *In-Package Chemistry Abstraction* (BSC 2003 [DIRS 161962]). The parameters abstracted in that document are pH, ionic strength, total carbonate, Eh, chloride, and fluoride. The uncertainty in the in-package chemistry due to different void volumes is small compared with that due to uncertainty in the waste package water inflow rates.

## **Supporting Documents:**

BSC 2003 [DIRS 161962]

#### **Related FEPs:**

2.1.09.01.0B, Chemical Characteristics of Water in Waste Package

## 6.2.15 Organic/Cellulosic Materials in Waste

#### **FEP Number:**

2.1.02.10.0A

**FEP Description**: Degradation of cellulose in the waste could affect the long-term performance of the disposal system.

## **Descriptor Phrases:**

Organic/cellulosic materials in waste

# **Screening Decision:**

Excluded (low consequence)

Screening Argument: Chemically reactive materials, such as cellulosic materials, are excluded from the repository (DOE 2002 [DIRS 158873], Sections 4.2.11, 4.3.1.B, 4.3.7.B, and 4.3.17) and only minor quantities of organic materials might appear as part of the waste (BSC 2003 [DIRS 161962]). Organic complexants, such as humic acid in groundwater, can cause actinide complexation at concentrations as low as one ppm. However, the quantities of humic materials in groundwater flowing into the drifts are not expected to be significant. In any case, actinide complexation in the drifts will not be significant (see FEP 2.1.09.13.0A). The minor amounts of organic materials in the emplaced waste and the insignificant complexation in the drifts will not result in any significant effects on repository performance. Therefore, this FEP can be excluded on the basis of low consequence to radiological exposures and radionuclide releases.

# **TSPA Disposition:**

N/A

#### **Supporting Documents:**

BSC 2003 [DIRS 161962]

## **Related FEPs:**

- 2.1.10.01.0A, Biologic Activity
- 2.1.12.04.0A, Gas Generation (CO<sub>2</sub>, CH<sub>4</sub>, H<sub>2</sub>S) from Microbial Degradation

# 6.2.16 DSNF Cladding

#### **FEP Number:**

2.1.02.25.0A

**FEP Description**: DSNF to be disposed of in Yucca Mountain has a variety of fuel types that may not be similar to the CSNF to be disposed. Some of the fuel types may have initial

cladding-degradation characteristics that are different from those for the CSNF. Therefore, the effectiveness of DSNF cladding as a barrier to radionuclide mobilization might be different from CSNF. This FEP addresses all types of DSNF cladding except naval SNF cladding.

## **Descriptor Phrases:**

Degradation of DSNF cladding

## **Screening Decision:**

Excluded (low consequence)

Screening Argument: More than 80 percent by weight of the DSNF is from the N-Reactor, a significant but unquantified fraction of which will have damaged cladding at the time of emplacement in their canisters (Abrefah et al. 1995 [DIRS 151125]). Up to 50 percent may be already perforated (Rechard 1995 [DIRS 101084], Section 11.3.1, pp. 11 to 24). There has been insufficient characterization of the condition of the DSNF cladding (other than the observations of extensive damage to the N-Reactor SNF cladding) to establish the effectiveness of the cladding as a barrier. Because the cladding integrity of most DSNF will not be extensively characterized (BSC 2003 [DIRS 163693], Section 6.4.3), the TSPA takes no credit for radionuclide containment by the cladding. Also, the TSPA takes no credit for canister integrity (i.e., once the waste package has leaked or failed); it is conservatively assumed that the DSNF is directly exposed to repository water or air environment. Because no credit will be taken for the cladding, mechanisms that might enhance cladding degradation do not impact the predicted consequences (CRWMS M&O 2000 [DIRS 153595]; Thornton 1998 [DIRS 107796]).

Additionally, postclosure site-boundary dose-sensitivity analyses have indicated that the increase of the dose rate at the site boundary resulting from the complete release of the radionuclide inventory in waste packages containing N-Reactor SNF during one performance assessment time step is insignificant (Thornton 1998 [DIRS 107796]). Since this represents over 80 percent of the DSNF inventory, not taking performance credit for the cladding the DSNF will provide a conservative estimate of the boundary dose. Also, the rate of unzipping of failed cladding can be conservatively assumed to be instantaneous in the TSPA-LA since the DSNF radionuclide inventory is small compared to the rest of the waste and the cladding is assumed not to provide a barrier anyway. Inclusion of the protective performance of DSNF cladding in the TSPA-SR calculation would reduce calculated doses.

Therefore, DSNF cladding degradation can be excluded from the TSPA-LA based on low consequence because it has no adverse effects on performance.

## **TSPA Disposition:**

N/A

# **Supporting Documents:**

BSC 2003 [DIRS 163693]

#### **Related FEPs:**

- 2.1.02.01.0A, DSNF Degradation (Alteration, Dissolution, and Radionuclide Release)
- 2.1.02.08.0A, Pyrophoricity From DSNF

## **6.2.17** Grouping of DSNF Waste Types into Categories

#### **FEP Number:**

2.1.02.28.0A

**FEP Description**: Several hundred distinct types of DOE-owned SNF (DSNF) may potentially be stored at YMP. These represent many more types than can viably be examined for their individual effect on the repository. A limited number of representative or bounding degradation models must be selected and/or abstracted. As a result, the effects on repository performance of the details related to the many distinct types of DSNF can not be evaluated.

## **Descriptor Phrases:**

N-Reactor fuel bounding model Naval fuel

## **Screening Decision:**

Included

## **Screening Argument:**

N/A

**TSPA Disposition**: DSNF to be disposed of in Yucca Mountain is composed of a variety of fuel types. The various DSNF types have been classified into eleven groups for the purpose of TSPA-LA analyses (DOE 2000 [DIRS 118968]). The largest single DSNF type is the N-Reactor SNF, which comprises approximately 84 percent by weight of the total DSNF. N-Reactor SNF uranium metal (Group 7) models are adopted as a surrogate for the entire DSNF inventory, except for the naval SNF (Group 1) (BSC 2003 [DIRS 163693]). The CSNF degradation model is used as the surrogate for naval SNF. This grouping and implementation simplifies the TSPA-LA model for computational efficiency while ensuring that the great majority of DSNF degradation is captured in a bounding fashion.

In addition to being the largest DSNF inventory type by weight, N-Reactor SNF degradation can be used to represent degradation of the entire DSNF inventory (Section 5.2.17 of this analysis report) because (1) a significant fraction of the N-Reactor SNF will be damaged at the time of emplacement in their canisters and (2) the N-Reactor SNF degradation model predicts dissolution rates greater than most other groups (BSC 2003 [DIRS 163693], Section 6.2 and Table 9). The group that potentially has greater dissolution rates than N-Reactor SNF is the mixed-carbide-fissile fuel waste particles in a nongraphite matrix (Group 3). Group 3 waste would not serve as an appropriate DSNF degradation surrogate because the total inventory of the Group 3 SNF is less than 0.001 percent of DSNF waste (DOE 2002 [DIRS 158405], Appendix D). The immobilized plutonium ceramic waste form is not included in this discussion because the DOE Office of Environmental Management has recently decided to use the majority of the excess defense plutonium as MOX fuel in commercial reactors as the preferred disposition path rather than immobilization in a ceramic waste form (67 FR 19432 [DIRS 162618]).

As discussed in *DSNF and Other Waste Form Degradation Abstraction* (BSC 2003 [DIRS 163693], Section 6.3), even when upper bound assumptions are used for N-Reactor SNF degradation rates (i.e., complete dissolution of the waste form during a single code time step

upon exposure of the waste form to groundwater) overall repository performance is insensitive to the DSNF degradation rate (Thornton 1998 [DIRS 107796]). Even under pyrophoric conditions (Thornton 1998 [DIRS 125082]), the contribution from DSNF is small because it is a small percent of the total waste, therefore waste stream plume chemistry is dominated by the CSNF waste even when bounding DSNF degradation models are used. Therefore, the categorization of DSNF waste into 11 groups and the use of N-Reactor SNF (Group 7) to represent, in a bounding fashion, the degradation rate of all DSNF (except naval SNF) is justified.

## **Supporting Documents:**

BSC 2003 [DIRS 163693]

#### **Related FEPs:**

- 2.1.02.01.0A, DSNF Degradation (Alteration, Dissolution, and Radionuclide Release)
- 2.1.02.25.0A, DSNF Cladding

#### 6.2.18 Flammable Gas Generation from DSNF

#### **FEP Number:**

2.1.02.29.0A

**FEP Description**: DOE-owned Spent Nuclear Fuel (DSNF) to be disposed of in Yucca Mountain will have a small percent of carbide fuel. When carbide is exposed to water, flammable gases such as methane and its minor constituents ethane, ethylene, and acetylene (referred to as ethyne by the International Union of Pure and Applied Chemistry) are generated. If these gases ignite, localized increases in temperature can occur, which might affect fuel degradation. The area around the ignition point may be mechanically and/or thermally perturbed, which could affect waste container or host-rock properties in the area of the EBS.

#### **Descriptor Phrases:**

Flammable gas (CH<sub>4</sub>)
Flammable gas (ethane, ethylene, acetylene)

## **Screening Decision:**

Excluded (low consequence)

**Screening Argument**: Flammable-gas generation from DSNF can be excluded based on low consequence for the following reasons:

1. The only fuel waste types capable of producing organic flammable gases such as methane, ethane, etc., are the U/Th carbide and the Pu/U carbide DSNF waste fuels because they are the only spent fuels containing more than trace quantities of carbon. These gases are formed by the reaction of the carbides with liquid water or water vapor. Only a small percentage (approximately 1 percent or 25 MTHM) of DSNF fuel contains U/Th carbide fuels and there is only about 100 kg of Pu/U carbide DSNF (DOE 2002 [DIRS 158405], Table D-1). Since DSNF comprises only about 4 percent of the total waste packages in the repository (DOE 2002 [DIRS 158405], Section 1), the carbide spent nuclear fuels will amount to less than 0.04 percent of the waste

packages. Additionally, all DNSF waste will be widely dispersed throughout the repository as will any produced flammable gas.

- 2. Additionally, the repository is located in fractured and unsaturated tuffaceous rock (DOE 2002 [DIRS 155943], Section 1.4.2.2.2). This rock is overlaid by approximately 250 meters of unsaturated welded and nonwelded tuffs. With the exception of intermittent perched zones, both the matrix and the fractures within the host rock above and below the repository horizon have a relatively high degree of gas saturation (generally greater than 50 percent), making these areas more gas-than liquid-permeable. Within the repository horizon, ambient gas saturation in the matrix ranges between 10 to 20 percent, while gas saturation in fractures tends to be much higher. These conditions will promote a dispersive gas flow path between the repository and host rock, thus diluting any potential flammable-gas concentrations to levels below the ignition point.
- 3. However, even if flammable gases were to accumulate and such an explosion were to occur, it would be small resulting in an insignificant release of radionuclides from the waste form. Consequently, the effect on radiological exposures to the reasonably maximally exposed individual and radionuclide releases to the accessible environment would not be significant.

The chemical reaction of U/Th carbide with water produces carbon dioxide and hydrocarbon gases. The major constituent of the hydrocarbon gases is methane, with minor constituents being ethane, ethylene, and acetylene. In sufficiently high concentrations, all of the hydrocarbon gases are flammable in air.

The Fort St. Vrain and Peach-Bottom Core-2 and Core 1 gas-cooled reactors used U/Th carbide fuel. Only the Peach-Bottom Core-1 reactor pellets are of concern, since pellets from this reactor are not encased in the tough, corrosion-resistant, silicon-carbide (SiC) shells, used in the other two reactors. Consequently many Peach-Bottom Core-1 pellets have broken open, with an estimated cladding failure rate of 35 percent (DOE 1998 [DIRS 122980], Appendix A, Section 6.9, p. 41). These pellets can possibly produce flammable hydrocarbons. Only 1.663 metric tons heavy metal (MTHM) of Peach Bottom Core 1 pellets (DOE 1998 [DIRS 122980], Appendix B, p. 14) contained in 103 waste packages (DOE 1998 [DIRS 122980], Table 1-1, p.1-8) will be disposed in the repository. This is small compared to the 24.667 MTHM of high-integrity fuel (contained in 545 waste packages) from the Fort St. Vrain and Peach-Bottom Core 2 reactors (DOE 1998 [DIRS 122980], Appendix B, p. 14 and Table 1-1, p.1-8). Thus, less than 7 percent  $\{1.663/(1.663 + 24.667)\}\$  of the carbide fuel is low-integrity pellets, of that only 2.5 percent (0.35 x 7 percent) is susceptible to gas production due to reaction with water. Taken all together only 0.001 percent (2.5 percent x 0.04 percent) of the waste to be disposed of in the repository is capable of producing flammable gases. Even if the cladding failure rate were 100 percent, only approximately 0.003 would be susceptible to gas production.

All DNSF waste will be codisposed among some 3,910 waste packages (DOE 2002 [DIRS 158405]; BSC 2003 [DIRS 161961], Table I-1), with one DSNF canister packaged per five CSNF canisters in each waste package. So the carbide fuel is inherently dispersed and any gas produced from carbide fuel would be dispersed as well. Furthermore, because the percent of

U/Th carbide waste is so small, any explosion from its gas product would be small resulting in an insignificant release of radionuclides from the waste form. This argument is further supported by an analysis of hydrocarbon production from carbide fuels (Propp 1998 [DIRS 149395]), concluding that hydrocarbon production is not a problem.

Changes to the fluid-flow characteristics of the flow system in the mountain could be produced by thermally driven mechanical and chemical processes. This could produce a condensation cap in some areas of the drift, reducing gas and water permeabilities, causing gas to possibly accumulate within the drift area. However, the probability of an ignition source being present is low. The possibility of reduced permeability to gas would also limit the availability of oxygen for combustion and greatly reduce the corrosion of containers, thereby reducing the number of containers potentially producing flammable or explosive gases. A condensation cap would reduce the influx of water contacting carbide U/Th waste, thus limit gas production from this source.

Additionally, flammable gases are not likely to accumulate in concentrations high enough to cause an explosion simply due to the physical setting of the repository. The repository is located in the unsaturated portion of the Topopah Spring Tuff, a fractured and welded unit. This unit is over- and underlain by other tuffaceous unsaturated units. Unsaturated Zone Flow and Transport Model Process Model Report (CRWMS M&O 2000 [DIRS 151940]) is a process model report generated for the Site Recommendation, and was cancelled for direct use in the TSPA-LA along with all Site Recommendation process model reports. However, that report's analyses of gas saturation are pertinent to this analysis. This is further supported by the unsaturated zone gas flow analyses by Simmons (2004 [DIRS 166960], Section 7.9.1.8). The matrix and the fractures above and below the repository horizon have a gas saturation generally greater than 50 percent (CRWMS M&O 2000 [DIRS 151940], Section 3.6), making these areas more gas- than liquid-permeable. In the repository horizon, gas saturation in the matrix varies from 10 to 30 percent (CRWMS M&O 2000 [DIRS 151940], Section 3.6), gas saturation in the fractures is much higher, causing gas to preferentially flow in the fractures. Consequently, any gas produced in the repository will tend to flow through the fracture complex with some gas diverted to the matrix at unit interfaces or where fracture networks pinch out (CRWMS M&O 2000 [DIRS 151940], Section 3.3). These flow paths will disperse flammable gas concentrations to levels below the ignition point. Additionally, airflow through Yucca Mountain maintains repository pressures within only a few pascals of atmospheric pressure. Given these conditions, any flammable gas produced, once released, will quickly disperse and be diluted due to the presence of in situ inert gases (nitrogen in the air, water vapor, and CO<sub>2</sub> and CH<sub>4</sub> from carbide reactions) in the repository.

# **TSPA Disposition:**

N/A

## **Supporting Documents:**

CRWMS M&O 2000 [DIRS 151940]

#### **Related FEPs:**

2.1.02.08.0A, Pyrophoricity From DSNF

## 6.2.19 Internal Corrosion of Waste Packages Prior To Breach

#### **FEP Number:**

2.1.03.06.0A

**FEP Description**: Aggressive chemical conditions within the waste package could contribute to corrosion from the inside out. Effects of different waste forms, including CSNF and DSNF, are considered in this FEP.

## **Descriptor Phrases:**

Internal corrosion of CSNF Internal corrosion of DSNF Chemical effects from radiolysis in-package

# **Screening Decision:**

Excluded (low consequence)

Screening Argument: It can be assumed that only a limited amount of water will be allowed by waste acceptance criteria inside a waste package (Section 5.2.19 of this analysis report), and there will be an inert gas backfill of waste packages and containers. Therefore, internal corrosion of waste packages prior to waste package breach can be excluded based on low consequence because only minor corrosion can occur within the low humidity environment of an unbreached package. Therefore, omission of minor internal corrosion of the waste package prior to breach will not significantly change the calculated radiological exposures and radionuclide releases. Radiolysis products could contribute to the interior corrosion, but they have been excluded based on low consequence. See FEP 2.1.13.01.0A.

Limited water is allowed in the CSNF and HLW-glass waste packages and that which exists initially will be rapidly consumed by reaction with the waste form. Consequently, prior to the breach of the waste packages, there should be little corrosion in the CSNF, DSNF, and HLW waste packages from normal chemical and water vapor mechanisms. Some DSNF-containing waste packages, such as those containing N-Reactor fuel, may have more water, but this water would be scavenged by the waste form due to the rapid corrosion rate of the metallic uranium that is the matrix of N-Reactor SNF compared with other SNF (BSC 2003 [DIRS 163693], Table 9; Gray and Einziger 1998 [DIRS 109691], Section 4), as well. After breach of the waste package, inside-out corrosion can be expected to add little to the net area through which fluids might enter the WF.

In general, no credit will be taken in the TSPA for DSNF canisters (within the waste package) as a barrier to fuel degradation and radionuclide mobilization. This decision was made because the canisters will be constructed of stainless steel, which will degrade relatively quickly once the waste package fails. Because no credit will be taken for the canisters, mechanisms that might enhance canister degradation do not impact the predicted consequences from the DSNF.

## **TSPA Disposition:**

N/A

## **Supporting Documents:**

BSC 2003 [DIRS 163693]

#### **Related FEPs:**

2.1.09.01.0B, Chemical characteristics of water in waste package

## 6.2.20 Chemical Characteristics of Water in Waste Package

## **FEP Number:**

2.1.09.01.0B

**FEP Description**: Chemical characteristics of the water in the waste packages (pH and dissolved species) may be affected by interactions with materials or steel used in the waste packages or waste forms and by the inflowing water from the drifts and near-field host rock.

The in-package chemistry, in turn may influence dissolution and transport as contaminants move through the waste, EBS, and down into the unsaturated zone.

## **Descriptor Phrases:**

Chemical effects from corrosion products in-package

Chemical effects from waste package degradation

Chemical effects from waste form degradation

Time-dependent THC characteristics in-package (temperature, pH, water concentration, gas concentration)

Inflowing water composition (into waste package)

Spatial heterogeneity of HLW glass degradation

#### **Screening Decision:**

Included

# **Screening Argument:**

N/A

**TSPA Disposition**: The chemical characteristics of water in the waste package are included in *In-Package Chemistry Abstraction* (BSC 2003 [DIRS 161962]). The IPCM is a fully coupled reaction-path chemical model which included the effects of waste-form dissolution, metal alloy corrosion/dissolution, precipitation of metal oxide corrosion products, precipitation of complex mineral phases, reaction kinetics, thermal effects, interior waste package void space, interactions of codisposed waste forms, oxidation–reduction reactions, heterogeneous chemical reactions, and seepage composition on the resulting fluid chemistry.

The variability in the initial chemistry of incoming water is included by considering three incoming water compositions in the IPCM. These compositions were then altered based on the corrosion rates of the steel components of the waste package internals and the seepage flux. These analyses resulted in a set of independent variables (steel corrosion rates, sulfur content of the WP inner barrier alloy A516, and the partial pressure of carbon dioxide) that were sampled to establish an uncertainty band for the determination of in-package chemistry. The outputs of the IPCM are time-varying aqueous inventories of fluid composition, reactant abundances, product

abundances, and solution properties. Solution parameters are abstracted into a TSPA-compatible format in *In-Package Chemistry Abstraction* (BSC 2003 [DIRS 161962]); therefore, all of the processes included in the IPCM are reflected in *In-Package Chemistry Abstraction* (BSC 2003 [DIRS 161962]) and thus in the TSPA. The IPCM parameters include pH, ionic strength, total carbonate, Eh, chloride, and fluoride.

## **Supporting Documents:**

BSC 2003 [DIRS 161962]

#### **Related FEPs:**

- 2.1.03.06.0A, Internal Corrosion of Waste Packages Prior to Breach
- 2.1.09.02.0A, Chemical Interaction With Corrosion Products
- 2.1.09.04.0A, Radionuclide Solubility, Solubility Limits, and Speciation in the Waste Form and EBS
- 2.1.09.06.0A, Reduction-Oxidation Potential in Waste Package

#### **6.2.21** Chemical Interaction with Corrosion Products

#### **FEP Number:**

2.1.09.02.0A

**FEP Description**: Corrosion products produced during degradation of the waste form, metallic portions of the waste package, and metals in the drift (rock bolts, steel in invert, gantry rails) may affect the mobilization and transport of radionuclides. Corrosion products may facilitate sorption/desorption and coprecipitation/dissolution processes. Corrosion products may form a "rind" around the fuel that could (1) restrict the availability of water for dissolution of radionuclides or (2) inhibit advective or diffusive transport of water and radionuclides from the waste form to the EBS. Corrosion products also have the potential to retard the transport of radionuclides to the EBS. Finally, corrosion products may alter the local chemistry, possibly enhancing dissolution rates for specific waste forms, or altering radionuclide solubility.

# **Descriptor Phrases:**

Colloid formation

Effects of corrosion products on waste form degradation

Time-dependent THC characteristics in-drift (solubility)

Chemical effects from corrosion products in-drift

Effects of corrosion products on waste package degradation

Chemical effects from corrosion products in-package

Time-dependent THC characteristics in-package (solubility)

#### **Screening Decision:**

Included

#### **Screening Argument:**

N/A

**TSPA Disposition**: The IPCM model developed in *In-Package Chemistry Abstraction* (BSC 2003 [DIRS 161962]) addresses in-package corrosion products and their effect on in-

package chemistry. The corrosion products of the steel and aluminum alloys in the waste package and their control on the concentration of aqueous species are of primary importance in determining the pH and ionic strength of the solution. If these corrosion products were not allowed to form during the simulations, then the resulting pH and ionic strength values would be much different than the results presented throughout Section 6.6 of *In-Package Chemistry Abstraction* (BSC 2003 [DIRS 161962]). Section 6.8 of *In-Package Chemistry Abstraction* (BSC 2003 [DIRS 161962]) examines the effect of surface complexation of aqueous species with waste package corrosion products and provides a pH range for in-package fluids to be used in TSPA-LA. The effects of interactions of corrosion products with the in-package chemistry are implicitly included in the abstractions passed to TSPA as part of *In-Package Chemistry Abstraction* (BSC 2003 [DIRS 161962]). The IPCM parameters include pH, ionic strength, total carbonate, Eh, chloride, and fluoride.

As described in *Waste Form and In-Drift Colloids-Associated Radionuclide Concentrations:* Abstraction and Summary (BSC 2003 [DIRS 166845]), fixed and suspended colloidal corrosion products are modeled in the waste package. Suspended colloidal corrosion products are modeled in the EBS. Corrosion colloids are assumed to form and are subject to concentration and stability constraints controlled by the aqueous chemistry. The potential development of rinds on fuel and glass waste surfaces has been implicitly included in the development of the colloid model by incorporating laboratory data derived from fuel and glass waste corrosion experiments. Clogging of waste package breached zones by corrosion products, as described in Section 6.3.1.3 of *Waste Form and In-Drift Colloids-Associated Radionuclide Concentrations: Abstraction and Summary* (BSC 2003 [DIRS 166845]), is addressed in FEP 2.1.03.10.0A (Healing of waste packages) in *FEPs Screening of Processes and Issues in Drip Shield and Waste Package Degradation* (BSC 2004 [DIRS 162200]).

The conceptual model and TSPA implementation for the colloidal radionuclide source term, developed from YMP-relevant data, include specific treatment of radionuclides associated with corrosion-product colloids formed during corrosion of waste package material and other metallic materials. In the TSPA-LA model, mass concentrations of corrosion product colloids are based on experimental observations on the degradation of miniature waste packages and iron oxide colloid concentrations observed in natural groundwaters within high iron-bearing geologic strata (BSC 2003 [DIRS 166845], Section 6.3.1.3). Aqueous chemical parameters, specifically ionic strength and pH, control the stability of the colloids. The model includes a provision for irreversible attachment of a fraction of Pu to corrosion-generated iron oxyhyrodroxide colloids and fixed corrosion mass (BSC 2003 [DIRS 166845], Section 6.3.3.2).

Model implementation of the following phenomena related to colloids and steel corrosion are described in *Waste Form and In-Drift Colloids-Associated Radionuclide Concentrations: Abstraction and Summary* (BSC 2003 [DIRS 166845]):

- Formation of iron oxyhydroxide colloids and fixed corrosion products in the waste package (Section 6.3.1.3);
- Estimation of stability and mass concentration of iron oxyhydroxide colloids from experimental results and calculated ionic strength and pH of in-package and in-drift fluids (Section 6.3.2.3);

- Irreversible sorption of Pu and Am onto iron oxyhydroxide colloids and fixed corrosion products (Section 6.3.3.2);
- Reversible sorption of dissolved Pu, Am, Pa, Th, and Cs onto iron oxyhydroxide colloids using developed K<sub>d</sub> values and the estimated colloid mass concentrations (Section 6.3.3.1).

The effects of dissolved iron on the glass dissolution rates are addressed by using the results of tests in which iron products were added to the test solution when determining model parameter values for pH dependence ( $\eta$ ) in acidic and alkaline solutions (BSC 2004 [DIRS 167619], Section 6.5.4.1). The effects of glass alteration phases on the glass dissolution rate are addressed by including the results of tests in which alteration phases and/or alteration product rinds form when determining model parameter values for  $k_E$  (BSC 2004 [DIRS 167619], Section 6.5.4.3).

# **Supporting Documents:**

BSC 2003 [DIRS 161962]

BSC 2003 [DIRS 166845]

BSC 2004 [DIRS 167619]

#### **Related FEPs:**

- 2.1.03.06.0A, Internal Corrosion of Waste Packages Prior to Breach
- 2.1.09.04.0A, Radionuclide Solubility, Solubility Limits, and Speciation in the Waste Form and EBS
- 2.1.09.06.0A, Reduction-Oxidation Potential in Waste Package
- 2.1.09.01.0B, Chemical Characteristics of Water in Waste Package

# 6.2.22 Radionuclide Solubility, Solubility Limits, and Speciation in the Waste Form and EBS

#### **FEP Number:**

2.1.09.04.0A

**FEP Description**: Degradation of the waste form will mobilize radionuclides in the aqueous phase. Factors to be considered in this FEP include the initial radionuclide inventory, justification of the limited inventory included in evaluations of aqueous concentrations, and the solubility limits for those radionuclides.

#### **Descriptor Phrases:**

Radionuclide solubility in-package Radionuclide solubility (concentration) limits Radionuclide speciation Radionuclide solubility in-drift

#### **Screening Decision:**

Included

## **Screening Argument:**

N/A

TSPA Disposition: Radionuclide solubility limits are also called dissolved concentration limits. Solubility models for 14 elements (plutonium, neptunium, uranium, thorium, americium, actinium, protactinium, radium, technetium, iodine, strontium, carbon, lead, and cesium) were developed, based on geochemical model calculations, where radionuclide speciation is considered, and documented in *Dissolved Concentration Limits of Radioactive Elements* (BSC 2003 [DIRS 163152]). Solubility models for these elements, except for lead, are included in the TSPA-LA model and used to constrain the maximum radionuclide concentrations in waste packages and in the invert. In the TSPA model, inventory concentrations of radioactive elements released from the waste forms (CSNF, DSNF, and HLW glass) are calculated according to the dissolution or degradation rates of waste forms and the volume of water within the (breached) waste package, and radionuclide inventory. Then, the inventory concentrations are compared against their solubility limits. The real concentrations available for transport are the lesser between the inventory concentrations and the solubility limits. If the inventory concentration is greater than its solubility limit, then the amount of that radioactive element in excess of the solubility limit will be kept in the inventory, and potentially available for transport at a later time.

For plutonium, neptunium, uranium, thorium, americium, actinium, and protactinium, solubilities are tabulated as functions of pH and log fCO<sub>2</sub> plus two or more uncertainty terms accounting for uncertainties associated with thermodynamic data, variations in water chemistry, and identification of solubility controlling solids (BSC 2003 [DIRS 163152], Sections 6.5 through 6.11). For radium and lead, solubilities are given as distributions or segmental constants (BSC 2003 [DIRS 163152]) Sections 6.12 and 6.13).

Under repository conditions, technetium, carbon, iodine and cesium are considered soluble and no solubility controlling solids are expected to form. Consequently, their releases are considered to be controlled by the dissolution rate of waste forms and the waste inventory (BSC 2003 [DIRS 163152], Sections 6.14 through 6.17). Strontium carbonate or sulfate may form under repository conditions, but they are quite soluble. Moreover, strontium does not contribute to dose significantly. Therefore, it is conservatively assumed that no strontium solubility-controlling solid exists and its release is considered to be controlled by the dissolution rate of waste forms and the waste inventory (BSC 2003 [DIRS 163152], Section 6.18).

## **Supporting Documents:**

BSC 2003 [DIRS 163152]

#### **Related FEPs:**

- 2.1.03.06.0A, Internal Corrosion of Waste Packages Prior to Breach
- 2.1.09.06.0A, Reduction-Oxidation Potential in Waste Package
- 2.1.09.01.0B, Chemical Characteristics of Water in Waste Package
- 2.1.09.02.0A, Chemical Interaction with Corrosion Products
- 2.1.09.08.0A, Diffusion of Dissolved Radionuclides in EBS
- 2.1.09.08.0B, Advection of Dissolved Radionuclides in EBS

## 6.2.23 Reduction-Oxidation Potential in Waste Package

#### **FEP Number:**

2.1.09.06.0A

**FEP Description**: The redox potential in the waste package influences the oxidation of waste form materials and the in-package solubility of radionuclide species. Local variations in the in-package redox potential can occur.

## **Descriptor Phrases:**

Time-dependent THC characteristics in-package (temperature, pH, water concentration, gas concentration)

## **Screening Decision:**

Included

## **Screening Argument:**

N/A

**TSPA Disposition**: *In-Package Chemistry Abstraction* (BSC 2003 [DIRS 161962]) bounds the redox potential of the groundwater seepage in the same equilibrium model that addresses the inpackage pH. The oxidation–reduction processes inside of the waste package are explicitly modeled in the IPCM and thus implicitly included in *In-Package Chemistry Abstraction* (BSC 2003 [DIRS 161962]). Oxidation of the metal waste package components is the primary process by which the waste packages corrode and the initial water composition is altered. In the absence of redox reactions there would be little alteration of the water inside of a failed waste package (BSC 2003 [DIRS 161962]).

The in-package chemistry abstraction shows that for CSNF waste packages there is some variability in the minerals and aqueous species in the reacted water chemistry of the water exiting a failed waste package for three different seepage compositions; J-13, "Na-porewater," and "Ca-porewater." (BSC 2003 [DIRS 161962], Table 2 and Section 6.6.1.2). However, this variability is small, and so the pH and ionic strength (redox potential) of the reacted solutions are unaffected by the variations in composition of the seepage water. Thus variability of the input water compositions, while included in TSPA-LA, are expected to have little or no effect on CSNF in-package chemistry.

For codisposed N-Reactor waste packages the mineral assemblages formed for the three seepage compositions indicate that the composition of the seepage water has little influence over which minerals will form and their amounts. Therefore, variability in the composition of water entering failed codisposed waste packages, while included in TSPA-LA, is expected to have little or no effect on the in-package chemistry (BSC 2003 [DIRS 161962], Section 6.6.2.2 and Figure 13).

The redox potential inside the waste package and its effect on in-package chemistry is implicitly included in the abstractions passed to TSPA as part of *In-Package Chemistry Abstraction* (BSC 2003 [DIRS 161962]). The IPCM parameters are pH, ionic strength, total carbonate, Eh, chloride, and fluoride.

## **Supporting Documents:**

BSC 2003 [DIRS 161962]

#### **Related FEPs:**

- 2.1.09.01.0B, Chemical Characteristics of Water in Waste Package
- 2.1.09.02.0A, Chemical Interaction with Corrosion Products

## **6.2.24** Reaction Kinetics in Waste Package

#### **FEP Number:**

2.1.09.07.0A

**FEP Description**: Chemical reactions, such as radionuclide dissolution/precipitation reactions and reactions controlling the reduction-oxidation state, may not be at equilibrium within the waste package.

## **Descriptor Phrases:**

Reaction path analysis using precipitation/dissolution rates Reaction path analysis using waste form degradation rates

## **Screening Decision:**

Included

## **Screening Argument:**

N/A

TSPA Disposition: Reaction kinetics and precipitation/dissolution rates are included in the TSPA-LA in-package chemistry model abstraction. The IPCM uses kinetic reactants to represent the SNF (BSC 2003 [DIRS 161962], Section 4.1.2) and the waste package components (BSC 2003 [DIRS 161962], Section 4.1.3.3). The kinetic rates used in the model were either linear, where a fixed amount of reactant is added at each time step, or a transition-state rate law where the amount of reactant added to the system depends on chemical properties of the aqueous phase. The effect of varying the kinetics on the in-package chemistry was examined (BSC 2003 [DIRS 161962], Section 6.7) where the rates were decreased to assess the contribution to uncertainty in pH and ionic strength for inclusion in the abstractions of pH for TSPA.

The variability in the kinetics of the reactants is included in the abstractions passed to TSPA both implicitly by their use in the IPCM, and explicitly via the contribution of the kinetics to output uncertainty. The effects of reaction kinetics on in-package chemistry are passed to TSPA as part of *In-Package Chemistry Abstraction* (BSC 2003 [DIRS 161962]). The IPCM parameters are pH, ionic strength, total carbonate, Eh, chloride, and fluoride.

#### **Supporting Documents:**

BSC 2003 [DIRS 161962]

#### **Related FEPs:**

- 2.1.09.06.0A Reduction-Oxidation Potential in Waste Package
- 2.1.09.01.0B, Chemical Characteristics of Water in Waste Package
- 2.1.09.02.0A, Chemical Interaction with Corrosion Products

## 6.2.25 Secondary Phase Effects on Dissolved Radionuclide Concentrations

#### **FEP Number:**

2.1.09.10.0A

**FEP Description**: Inclusion of radionuclides in secondary uranium mineral phases, such as neptunium in schoepite and uranium silicates, could affect radionuclide concentrations in water in contact with the waste form. During radionuclide alteration, the radionuclides could be chemically bound to immobile compounds and result in a reduction of radionuclides available for mobilization.

## **Descriptor Phrases:**

Secondary phase effects on dissolved radionuclide concentrations in-package Secondary phase effects on dissolved radionuclide concentrations in-drift

## **Screening Decision:**

Excluded (low consequence)

Screening Argument: Incorporation of certain radionuclide(s) into corrosion products formed during the alteration of spent nuclear fuel may reduce radionuclide concentrations in waters that have contacted fuel and its corrosion products (BSC 2003 [DIRS 163152], Section 6.3.2). It is well known that measured actinide concentrations in spent nuclear fuel corrosion experiments are several orders of magnitude lower than calculated solubilities assuming pure phase control (e.g., Werme and Spahiu 1998 [DIRS 113466], Chen 2001 [DIRS 161997]). This large discrepancy was attributed to the incorporation of actinides into secondary uranium phases (e.g., Werme and Spahiu 1998 [DIRS 113466]; Quinones et al. 1996 [DIRS 161925]; Chen 2001 [DIRS 161997]; Chen et al. 2002 [DIRS 161996]), which was not accounted for in conventional solubility calculations.

It can be assumed (Section 5.2.25 of this analysis report) that the constant ratio of neptunium to uranium in the leachate is the result of the formation of solid solutions in the secondary uranium phases. Three lines of evidence support the incorporation explanation. First, Burns et al. (1997 [DIRS 100389]) predicted that "the substitutions  $Pu^{6+} \leftrightarrow U^{6+}$  and  $(Np^{5+}, Pu^{5+}) \leftrightarrow U^{6+}$  are likely to occur in most  $U^{6+}$  structures" based on an analysis of the crystal–chemical properties of the U–O bond, Np–O bond, and Pu–O bond.

The previous theoretical prediction has been confirmed by direct observations of neptunium in uranyl minerals. Buck et al. (1998 [DIRS 100388]) examined corrosion products of spent nuclear fuel drip tests by electron energy loss spectroscopy analyses in a transmission electron microscope. As reported in their study, neptunium was to be incorporated into dehydrated schoepite (UO<sub>3</sub> · 0.8H<sub>2</sub>O) or metaschoepite (UO<sub>3</sub> · 2H<sub>2</sub>O). Finch et al. (2002 [DIRS 161979]) also reported experimental results on neptunium incorporation into dehydrated schoepite and estimated that the amount of neptunium incorporated in dehydrated schoepite can be as high as 2 percent of the host solid based on electron energy loss spectroscopy measurement. However, Finch has since questioned the reliability of the electron energy loss spectroscopy measurement (Adkins 2003 [DIRS 163864]).

More significant progress in this direction is the successful synthesis of neptunium-bearing uranium minerals. Burns et al. (1997 [DIRS 100389]) reported the synthesis of uranophane (Ca(UO<sub>2</sub>SiO<sub>3</sub>OH)<sub>2</sub> · 5H<sub>2</sub>O) and Na-compreignacite (Na<sub>2</sub>[(UO<sub>2</sub>)<sub>3</sub>O<sub>2</sub>(OH)<sub>3</sub>]<sub>2</sub>(H<sub>2</sub>O)<sub>5</sub>) containing neptunium ranging up to 497 ppm (Buck et al. 2003 [DIRS 168411]). Furthermore, they found that "there is a linear relationship between the neptunium content of α-uranophane and Nacompreignacite and the Np<sup>5+</sup> concentration in the initial solution," and "Np is incorporated into crystals of alpha-uranophane and Np-compreignacite in approximately the same concentrations as presented in the mother solutions." Buck (2003 [DIRS 168411]), Friese et al. (2003 [DIRS 162634]), and Friese (2003 [DIRS 163911]) also reported the successful synthesis of neptuniumbearing studtite (UO<sub>4</sub>·4H<sub>2</sub>O). In the neptunium incorporation experiments conducted by Burns et al. (Buck et al. 2003 [DIRS 168411]), it is found that schoepite, the major secondary uranyl mineral that forms in the process of spent nuclear fuel degradation and believed to be critical for neptunium immobilization, contains only a small amount of neptunium (a few parts per million). Burns et al. attribute this to the lack of suitable low-valence cations in their experiments (Buck et al. 2003 [DIRS 168411]). This may have prevented a charge-balance mechanism from happening, which is a prerequisite for neptunium incorporation into uranyl minerals. Burns et al. planned to conduct experiments using various counter ions (potassium, cesium, and calcium, etc.) to examine their effects on neptunium incorporation into schoepite (Buck et al. 2003 [DIRS 1684111).

Finally, Chen (2001 [DIRS 161997]) and Chen et al. (2002 [DIRS 161996]) analyzed the relative release rates of neptunium and uranium in the fuel degradation experiments referred to above and found a close correlation between neptunium and uranium concentrations in the leachates. In other words, the ratio of neptunium to uranium in the leachate is equal to the ratio in the spent nuclear fuel used in the experiments. Bruno et al. (1998 [DIRS 101565]) have also observed a coherent relation between neptunium and uranium in spent nuclear fuel dissolution experiments in the Spanish Nuclear Waste Program. These results are corroborated by the linear relationship between neptunium contents in uranophane and Na-compreignacite and the mother solution that was found by Burns et al. (Buck et al. 2003 [DIRS 168411]).

There are several conceivable explanations for this coherent relation between neptunium and uranium. First, it is the result of congruent dissolution of fuel matrix with few effects of secondary phases. The second explanation is that neptunium and uranium behave coherently, not only in the dissolution process but also in the process of secondary phase precipitation. The third entails uranium and neptunium self-formed solid phases controlling their associated solubilities at a ratio equal to that of uranium to neptunium in the fuel. However, only one explanation is reasonable. The first can be eliminated because a large portion of reacted uranium precipitated as secondary uranium minerals; therefoe, they are incongruent reactions. The third hypothesis relies on coincidence and, as stated earlier, no neptunium pure phases have been reported in fuel dissolution experiments; thus, it is unsubstantiated. Therefore, the second explanation is the most reasonable. In other words, the coherent relation between neptunium and uranium is the result of formation of solid solutions between neptunium and uranium.

A mechanistic model was developed (CRWMS M&O 1998 [DIRS 100362]; Chen et al. 1999 [DIRS 145441]; Chen 2003 [DIRS 162709]) that assumed neptunium is incorporated into secondary uranyl minerals (Section 5.2.25 of this analysis report), based on experimental observations that the neptunium and uranium behave coherently in the release from the waste

form and in the secondary phase formation process. The reactive-transport model considers equilibrium reactions and kinetic dissolution or precipitation reactions of solids under flow conditions. The modeling results were compared against laboratory measurements and observations of natural analogs. For repository conditions, the model predicted neptunium solubility ranges from  $1.0 \times 10^{-9}$  to  $1.0 \times 10^{-6}$  mol/L, about two orders of magnitude lower than the value used for the TSPA-VA base case. A TSPA sensitivity study used this solubility range and showed that the peak neptunium dose rate was reduced by a factor of 45 from the base case (DOE 1998 [DIRS 100550], Section 5.5.3).

An alternative model of accounting for incorporation of neptunium into uranyl minerals was generated based on experimental data. The results produced by the alternative model captures experimental results well (BSC 2003 [DIRS 163152], Section 6.6.4.5). It eliminates the built-in conservatism in the conventional pure phase solubility approach and, thus, gives more realistic source terms. However, experimental studies on whether schoepite, the critical secondary uranyl phase, can incorporate and immobilize sufficient neptunium during spent nuclear fuel corrosion do not provide a solid basis for recommending this model to be used in the TSPA-LA model. Experimental work leading to data bearing on this model is under continuous review and may lead to an amended recommendation to adopt neptunium concentrations based on the coprecipitation model.

In summary, although the inclusion of secondary-mineral phases in the TSPA-LA would reduce calculated doses because these solids have the ability to sequester radionuclides, no credit is taken for this process in the TSPA-LA. Therefore, secondary-phase effects on dissolved radionuclide concentrations are excluded from the TSPA-LA based on low consequence because they have no adverse effects on performance.

## **TSPA Disposition:**

N/A

#### **Supporting Documents:**

BSC 2003 [DIRS 163152]

## **Related FEPs:**

- 2.1.09.06.0A, Reduction—Oxidation Potential in Waste Package
- 2.1.09.01.0B, Chemical Characteristics of Water in Waste Package
- 2.1.09.02.0A, Chemical Interaction with Corrosion Products

# **6.2.26** Complexation in EBS

## **FEP Number:**

2.1.09.13.0A

**FEP Description**: The presence of organic complexants in water in the EBS could augment radionuclide transport by providing a transport mechanism in addition to simple diffusion and advection of dissolved material. Organic complexants may include materials found in natural groundwater such as humates and fulvates, or materials introduced with the waste or engineered materials

## **Descriptor Phrases:**

Complexation in EBS

# **Screening Decision:**

Excluded (low consequence)

**Screening Argument**: Repository temperatures are expected to remain sufficiently high to prevent water condensation and consequent formation of media for organic activity for several thousand years. Once lower temperatures recur, microbial populations will not be sufficient to generate significant concentrations of radionuclide-chelating organics. Organic complexants are typically found in sufficient quantity to move radionuclides long distances only in organic rich soils and groundwaters – or downgradient from dumps containing high levels of organic matter. Bounding biomass estimates for the repository are approximately 100 grams (dry) per meter of drift (CRWMS M&O 2000 [DIRS 151561], Table 71 and Section 7.2), several orders of magnitude below the cases cited above and insufficient to produce high chelate levels. Note, moreover, that many organic complexants also complex with multivalent nonradioactive metal cations, such as Fe(III) and Ni(II), will be present in much higher concentrations than the actinides (BSC 2001 [DIRS 162733]). This would also inhibit wide-scale complexation of actinides by organic matter. Also, the estimates of microbe masses growing in the repository system suggest that the effects on the bulk in-drift geochemistry should be small (CRWMS M&O 2000 [DIRS 151561], p. 154), and that these colloids are accounted for as well in the dissolved concentrations model report (BSC 2003 [DIRS 163152]). In conclusion, the magnitude and time of the resulting radiological exposures to the reasonably maximally exposed individual, or radionuclide releases to the accessible environment, are not significantly changed by the omission of this FEP from the TSPA-LA.

## **TSPA Disposition:**

N/A

## **Supporting Documents:**

CRWMS M&O 2000 [DIRS 151561] BSC 2001 [DIRS 162733] BSC 2003 [DIRS 163152]

#### **Related FEPs:**

- 2.1.09.06.0A, Reduction-Oxidation Potential in Waste Package
- 2.1.09.01.0B, Chemical Characteristics of Water in Waste Package
- 2.1.09.02.0A, Chemical Interaction with Corrosion Products

#### 6.2.27 Formation of True (Intrinsic) Colloids in EBS

#### **FEP Number:**

2.1.09.15.0A

**FEP Description**: True colloids are colloidal-sized assemblages (between approximately 1 nanometer and 1 micrometer in diameter) consisting of hydrolyzed and polymerized radionuclides. They may form in the waste package and EBS during waste-form degradation and radionuclide transport. True colloids are also called primary colloids, real colloids, Type I

colloids, Eigenkolloide, and intrinsic colloids (or actinide intrinsic colloids, for those including actinide elements).

# **Descriptor Phrases:**

Formation of true (intrinsic) colloids in EBS

## **Screening Decision:**

Excluded (low consequence)

Screening Argument: Saturated solutions in close proximity to degrading waste may form true colloids (BSC 2003 [DIRS 166845], Section 6.3.1). However, true colloids may not be routinely detectable, as they are difficult to distinguish from dissolved radionuclides. Further, they would be likely to dissociate in dilute fluids typical of the repository as well as sorb to substrates. Uranium colloids that have been observed to form are meta-schoepite or other oxyhydroxides that are soluble in the dilute oxic waters expected in the unsaturated and saturated zone environments. Consequently, these colloids will eventually dissolve, in part because of their small size and large reactive surface area, and in part because of increasingly dilute groundwater conditions away from the near field (BSC 2003 [DIRS 166845], Sections 6.3.1.2 and 6.3.1.2.1 through 6.3.1.2.4).

Uranium is modeled in the EBS as U-aqueous complexes not associated with colloids (BSC 2003 [DIRS 166845], Sections 6.3.1.2.1, 6.3.1.2.2, and 6.3.1.2.4). Any uranium that might form metastable true colloids and then subsequently dissolve is already considered as part of these U-aqueous complexes. The mass of uranium that might potentially form metastable true colloids is not expected to be significant with respect to the total mass of radionuclides, nor is the enhanced colloid transport in the EBS of those potential true colloids significant with respect to the total transport time to the accessible environment. Therefore, the impact of true colloids on radiological exposures to the reasonably maximally exposed individual and radionuclide releases to the accessible environment would not be significant.

In summary, true colloids, even if they were to form, would be metastable and would dissolve in the dilute waters away from the waste package. In their metastable form in the EBS, they would not have a significant effect on transport. Therefore, the formation of true colloids in the EBS has been excluded from the TSPA-LA on the basis of low consequence.

#### **TSPA Disposition:**

N/A

## **Supporting Documents:**

BSC 2003 [DIRS 166845]

### **Related FEPs:**

- 2.1.09.16.0A, Formation of Pseudocolloids (Natural) in EBS
- 2.1.09.17.0A, Formation of Pseudocolloids (Corrosion Product) in EBS
- 2.1.09.18.0A, Formation of Microbial Colloids in EBS
- 2.1.09.23.0A, Stability of Colloids in EBS
- 2.1.09.25.0A, Formation of Colloids (Waste-Form) by Coprecipitation in EBS
- 2.1.09.19.0B, Advection of Colloids in EBS
- 2.1.09.24.0A, Diffusion of Colloids in EBS

## 6.2.28 Formation of Pseudo-Colloids (Natural) in EBS

#### **FEP Number:**

2.1.09.16.0A

**FEP Description**: Pseudo-colloids are colloidal-sized assemblages (between approximately 1 nanometer and 1 micrometer in diameter) of nonradioactive material that have radionuclides bound or sorbed to them. Natural pseudo-colloids include microbial colloids, mineral fragments (clay, silica, iron oxyhydroxides), and humic and fulvic acids. This FEP addresses radionuclide-bearing pseudocolloids formed from host-rock materials and all interactions of the waste and EBS with the host rock environment except corrosion.

### **Descriptor Phrases:**

Natural groundwater colloids (clay, silica, iron oxyhydroxide, invert/tuff)

## **Screening Decision:**

Included

### **Screening Argument:**

N/A

**TSPA Disposition**: Natural colloids are modeled as smectite clay colloids as discussed in *Waste Form and In-Drift Colloids-Associated Radionuclide Concentrations: Abstraction and Summary* (BSC 2003 [DIRS 166845], Section 6.3.1.4). Pseudocolloids generally form as a result of dissolved (aqueous) radionuclides sorbing to existing colloids (BSC 2003 [DIRS 166845], Section 6.3.1). K<sub>d</sub> values are developed to model reversible sorption of Pu, Am, Th, Pa, and Cs onto smectite groundwater colloids to form pseudocolloids (BSC 2003 [DIRS 166845], Section 6.3.3.1). Stability of the colloids is determined based on ionic strength and pH; concentration is modeled as a sampled parameter based on field observations in the Yucca Mountain vicinity (BSC 2003 [DIRS 166845], Sections 6.3.2.2 and 6.3.2.5). Sorption to iron oxyhydroxide colloids is also modeled, with implementation in TSPA-LA simplified by using one set of K<sub>d</sub> values. Glass waste form colloids are also modeled as smectite clay colloids, based on experimental observations at ANL, and are modeled to respond to ionic strength and pH conditions in the same manner as natural groundwater colloids (see FEP 2.1.09.25.0A).

### **Supporting Documents:**

BSC 2003 [DIRS 166845]

### **Related FEPs:**

- 2.1.09.15.0A, Formation of True (Intrinsic) Colloids in EBS
- 2.1.09.17.0A, Formation of Pseudocolloids (Corrosion Product) in EBS
- 2.1.09.18.0A, Formation of Microbial Colloids in EBS
- 2.1.09.23.0A, Stability of Colloids in EBS
- 2.1.09.25.0A, Formation of Colloids (Waste-Form) by Coprecipitation in EBS
- 2.1.09.19.0B, Advection of Colloids in EBS
- 2.1.09.24.0A, Diffusion of Colloids in EBS

### 6.2.29 Formation of Pseudocolloids (Corrosion Product) in EBS

#### **FEP Number:**

2.1.09.17.0A

**FEP Description**: Pseudocolloids are colloidal-sized assemblages (between approximately 1 nanometer and 1 micrometer in diameter) of nonradioactive material that have radionuclides bound or sorbed to them. Corrosion product pseudocolloids include iron oxyhydroxides from corrosion and degradation of the metals in the EBS and silica from degradation of cementitious materials.

# **Descriptor Phrases:**

Corrosion product colloids (metal oxyhydroxide, iron oxides, and cement grout silica)

# **Screening Decision:**

Included

### **Screening Argument:**

N/A

**TSPA Disposition**: The TSPA-LA model abstraction (BSC 2003 [DIRS 166845]) includes treatment of radionuclides associated with corrosion of steel components of the waste package and surrounding drift materials. Fixed and colloidal corrosion products are modeled in the waste package (BSC 2003 [DIRS 166845], Section 6.3.3.2). Colloids formed from the corrosion of steel in the EBS are modeled as iron oxyhydroxide colloids, with estimated mass concentrations based on corrosion studies of miniature waste packages under YMP-relevant conditions and iron oxide colloid concentrations observed in groundwaters associated with high iron-bearing geologic strata (BSC 2003 [DIRS 166845], Section 6.3.1.3).

Pseudocolloids generally form as a result of dissolved (aqueous) radionuclides sorbing to existing colloids (Section 6.3.1). K<sub>d</sub> values were developed to model reversible sorption of Pu, Am, Th, Pa, and Cs onto iron oxyhydroxide corrosion colloids to form pseudocolloids (BSC 2003 [DIRS 166845], Section 6.3.3.1). In addition, Pu and Am are modeled as sorbing irreversibly to iron oxyhydroxide corrosion colloids (BSC 2003 [DIRS 166845], Section 6.3.3.2).

Iron oxyhydroxide corrosion colloids are subject to concentration and stability constraints controlled by the aqueous chemistry, chiefly determined from the ionic strength and pH of inpackage and in-drift fluids (BSC 2003 [DIRS 166845], Section 6.3.2.3).

In the TSPA-LA model, a major fraction (approximately 0.9 or higher) of sorbed Pu is assumed to become irreversibly attached to corrosion products (stationary corrosion materials and iron oxyhydroxide colloids). The remainder is assumed to become reversibly attached according to an appropriate K<sub>d</sub> (BSC 2003 [DIRS 166845], Section 6.3.3.1, Table 10). This capability was included to acknowledge laboratory and field observations that the attachment of a large fraction of Pu to iron oxyhydroxide persists over the time of the observations and dissolved Pu concentrations are small, as observed in natural groundwater systems, because Pu is strongly sorbed onto stationary geologic media and colloids.

## **Supporting Documents:**

BSC 2003 [DIRS 166845]

#### **Related FEPs:**

- 2.1.09.15.0A, Formation of True (Intrinsic) Colloids in EBS
- 2.1.09.16.0A, Formation of Pseudocolloids (Natural) in EBS
- 2.1.09.18.0A, Formation of Microbial Colloids in EBS
- 2.1.09.23.0A, Stability of Colloids in EBS
- 2.1.09.25.0A, Formation of Colloids (Waste-Form) by Coprecipitation in EBS
- 2.1.09.19.0B, Advection of Colloids in EBS
- 2.1.09.24.0A, Diffusion of Colloids in EBS

### 6.2.30 Formation of Microbial Colloids in EBS

#### **FEP Number:**

2.1.09.18.0A

**FEP Description**: This FEP addresses the formation and transport of microbial colloids in the waste and EBS.

## **Descriptor Phrases:**

Microbial colloids

### **Screening Decision:**

Excluded (low consequence)

**Screening Argument**: The effects of colloid-facilitated radionuclide transport stemming from biological activity have been excluded from the TSPA-LA model analysis. The potential influence of organic complexants from microbial metabolism on radionuclide transport is assumed (Section 5.2.30) not to affect the stability of inorganic (mineral) colloids (BSC 2003 [DIRS 166845], Sections 5.9 and 6.3.4) (i.e., inorganic colloid stability is determined by fluid chemistry [ionic strength and pH]). Because inorganic aqueous conditions dominate DHLWG degradation rates, and microbial degradation is secondary, this process is excluded on the basis of low consequence.

Microbe-induced reduction of radionuclide, metal, and sulfate contaminants would decrease their mobility (BSC 2003 [DIRS 166845], Section 6.3.4), which is beneficial to performance. Biofilms would tend to retard radionuclides, which is also beneficial. These beneficial processes can be excluded from the TSPA-LA on the basis of low consequence because they have no

adverse effects on performance (i.e., their influence would not lead to increased potential dose as their activity has been deemed to promote colloid instability and reduced transport of radionuclides in association with colloids).

For microbes to impact near-field performance, microbes must be present and sufficient energy sources and nutrients must be available. For microbes to have an unfavorable impact on performance, they must accumulate radionuclides and must be transportable. Because of the relatively large microbes, they will be readily filtered during transport, along with any accumulated radionuclides, which is beneficial. Inclusion of microbial colloid transport in the waste and EBS would reduce calculated doses, and thus be potentially nonconservative. It is reasonable to conclude that the presence of organic polymers such as those produced by microbes and their byproducts will generally reduce the stability of inorganic colloids and result in enlargement of particles through heteroaggregation. It is also reasonable to conclude that microbes in the repository environment would likewise decrease the mobility and stability of colloids.

Consequently, this FEP can be excluded based on low consequence.

# **TSPA Disposition:**

N/A

### **Supporting Documents:**

BSC 2003 [DIRS 166845]

#### **Related FEPs:**

- 2.1.09.15.0A, Formation of True (Intrinsic) Colloids in EBS
- 2.1.09.16.0A, Formation of Pseudocolloids (Natural) in EBS
- 2.1.09.17.0A, Formation of Pseudocolloids (Corrosion Product) in EBS
- 2.1.09.23.0A, Stability of Colloids in EBS
- 2.1.09.25.0A, Formation of Colloids (Waste-Form) by Coprecipitation in EBS
- 2.1.09.19.0B, Advection of Colloids in EBS
- 2.1.09.24.0A, Diffusion of Colloids in EBS

### 6.2.31 Stability of Colloids in EBS

#### **FEP Number:**

2.1.09.23.0A

**FEP Description**: For radionuclide-bearing colloids to affect repository performance, the colloids in the dispersion must remain suspended, that is, be stable, for time scales that are long relative to time required for groundwater transport. Further, they must carry significant concentrations of radionuclides. The stability of smectite colloids, which is applicable for YMP groundwater colloids and waste-form colloids, is determined primarily by ionic strength but also to an extent by pH. The stability of iron oxyhydroxide colloids, which is applicable to corrosion-product colloids, is determined by both ionic strength and pH.

## **Descriptor Phrases:**

Time-dependent THC characteristics in EBS (pH, ionic strength)

### **Screening Decision:**

Included

### **Screening Argument:**

N/A

**TSPA Disposition**: Colloids in the EBS modeled in *Waste Form and In-Drift Colloids-Associated Radionuclide Concentrations: Abstraction and Summary* (BSC 2003 [DIRS 166845]) are smectite (waste form and groundwater colloids) and iron oxyhydroxide (steel corrosion colloids). Their stabilities are determined from ionic strength and pH of the in-package and in-drift fluids, as calculated in the TSPA-LA model calculations.

The stabilities of both smectite and iron hydroxide colloids are determined at each time step executed in the TSPA-LA calculations (BSC 2003 [DIRS 166845], Section 6.3.2). These determinations are then used to calculate concentrations of radionuclides associated with the colloids (BSC 2003 [DIRS 166845], Section 6.3.3). Ionic strength, pH values, and dissolved radionuclide concentrations are taken from intermediate TSPA-LA calculation values from submodels described in the in-package chemistry waste package (ionic strength and pH), solubility limits (dissolved radionuclides), and near-field chemical environment (drift ionic strength and pH) model reports (BSC 2003 [DIRS 166845], Section 6.5).

# **Supporting Documents:**

BSC 2003 [DIRS 166845]

### **Related FEPs:**

- 2.1.09.15.0A, Formation of True (Intrinsic) Colloids in EBS
- 2.1.09.16.0A, Formation of Pseudocolloids (Natural) in EBS
- 2.1.09.17.0A, Formation of Pseudocolloids (Corrosion Product) in EBS
- 2.1.09.18.0A, Formation of Microbial Colloids in EBS
- 2.1.09.25.0A, Formation of Colloids (Waste-Form) by Coprecipitation in EBS
- 2.1.09.19.0B, Advection of Colloids in EBS
- 2.1.09.24.0A, Diffusion of Colloids in EBS

### 6.2.32 Formation of Colloids (Waste-Form) by Coprecipitation in EBS

#### **FEP Number:**

2.1.09.25.0A

**FEP Description**: Dissolved radionuclides and other ions may coprecipitate to form colloids. Coprecipitates may consist of radionuclides bound in the crystal lattice of a dominating mineral phase or may consist of radionuclides engulfed by a dominating mineral phase.

### **Descriptor Phrases:**

Waste form colloids (HLW glass)

## **Screening Decision:**

Included

### **Screening Argument:**

N/A

**TSPA Disposition**: Colloids apparently formed from coprecipitation of smectite and embedded radionuclide-bearing phases were observed in the DHLWG degradation tests (BSC 2003 [DIRS 166845], Section 6.3.1.1). Colloids produced from degradation of DHLWG are modeled as smectite colloids with "embedded" (assumed permanently attached) radionuclides, Pu and These may, in a broad sense, be considered coprecipitates. The concentrations of radionuclides associated with those colloids are based on empirical results from YMP-relevant DHLWG corrosion experiments (BSC 2003 [DIRS 166845], Sections 6.3.1.1 and 6.3.2.4). Mass concentrations of the colloids are based on those experiments with consideration of colloid mineralogy and the effects of ionic strength and pH on the stability of the colloids (BSC 2003 [DIRS 166845], Sections 6.3.1.1, 6.3.2.2, and 6.3.2.4). Radionuclides associated with these colloids are modeled in the TSPA-LA model as "irreversibly attached" because they are embedded within the colloid matrix and can only be released upon the dissolution of the colloid. However, radionuclides within the aqueous environment can reversibly attach to the surfaces of these colloids and these colloid-radionuclide complexes can, therefore, be subject to transport in the TSPA-LA model as pseudocolloids. Radionuclide sorption onto these pseudocolloids is modeled by assigning Kd values developed to model reversible sorption of Pu, Am, Th, Pa, and Cs onto smectite colloids (BSC 2003 [DIRS 166845], Section 6.3.3.1). Similar to natural groundwater smectite colloids, the pseudocolloid stability is controlled by ionic strength and pH.

## **Supporting Documents:**

BSC 2003 [DIRS 166845]

### **Related FEPs:**

- 2.1.09.15.0A, Formation of True (Intrinsic) Colloids in EBS
- 2.1.09.16.0A, Formation of Pseudocolloids (Natural) in EBS
- 2.1.09.17.0A, Formation of Pseudocolloids (Corrosion Product) in EBS
- 2.1.09.18.0A, Formation of Microbial Colloids in EBS
- 2.1.09.23.0A, Stability of Colloids in EBS
- 2.1.09.25.0A, Formation of Colloids (Waste-Form) by Coprecipitation in EBS
- 2.1.09.19.0B, Advection of Colloids in EBS
- 2.1.09.24.0A, Diffusion of Colloids in EBS

#### **6.2.33** Exothermic Reactions in EBS

### **FEP Number:**

2.1.11.03.0A

**FEP Description**: Exothermic reactions liberate heat and will alter the temperature of the disposal system and affect the properties of the repository and surrounding materials. Oxidation of uranium metal fuels such as represented by N-Reactor fuels is one example of a possible exothermic reaction. Hydration of concrete used in the underground environment is another example of a possible exothermic reaction in the EBS.

### **Descriptor Phrases:**

Oxidation of uranium metal fuel Hydration of concrete Pyrophoricity

## **Screening Decision:**

Excluded (low consequence)

**Screening Argument**: Exothermic reactions, and other thermal reactions, that liberate heat in the waste and EBS are excluded from the TSPA because the possible temperature rise in a disposal container from an exothermic degradation of waste such as N-Reactor uranium metal in DSNF, or in the EBS from the hydration of concrete, is negligible in comparison to the substantial heat generated by radioactive decay. For example, the heat of reaction by oxidizing all N-Reactor fuel uranium metal is roughly 1.3 x 10<sup>13</sup>J, or 1/100th the heat energy produced in one year by all DSNF and HLW (where DSNF and HLW amount to approximately 7,000 MTHM, or one-tenth of the total repository mass of 70,000 MTHM) (DOE 1998 [DIRS 122980]), Section ES.3.4).

In addition, the conservative degradation rates used for DSNF already bound any additional thermally induced degradation effects that might result from exothermic reactions in the DSNF (see Section 6.2.6, FEP 2.1.02.01.0A). Because there is no temperature dependence in the recommended upper-limit DSNF model and because the degradation model is complete degradation within the first time step after contact by water, an increase in degradation rate due to temperature increase will have no impact on dose calculations. TSPA calculations will not be sensitive to differences within a TSPA time step. Note as well that the related effects of pyrophoric reactions are also excluded (See Section 6.2.13, FEP 2.1.02.08.0A).

Therefore, this FEP can be excluded based on low consequence to radiological exposures to the reasonably maximally exposed individual and radionuclide releases to the accessible environment.

### **TSPA Disposition:**

N/A

### **Supporting Documents:**

N/A

### **Related FEPs:**

- 2.1.02.01.0A, DSNF Degradation (Alteration, Dissolution, and Radionuclide Release)
- 2.1.02.08.0A, Pyrophoricity From DSNF

### 6.2.34 Thermal Effects on Chemistry and Microbial Activity in the EBS

#### **FEP Number:**

2.1.11.08.0A

**FEP Description**: Temperature changes may affect chemical and microbial processes in the waste and EBS.

### **Descriptor Phrases:**

Thermal effects on in-drift chemistry Thermal effects on in-package chemistry

### **Screening Decision:**

Included

### **Screening Argument:**

N/A

**TSPA Disposition**: Thermal effects may have an important influence on the rate of water contact with either the waste package, drip shield, or both (thereby influencing the corrosion rate), and on the rate of water influx into a failed waste package (thereby influencing the rate of waste form dissolution). Examples include localized dryout in the immediate vicinity of the waste packages during the early thermal phase of the repository history, as well as evaporation condensation on the underside of the drip shield providing an additional source term of water for dripping onto the waste package. Thermal effects on gaseous, liquid, or two-phase flow within the waste and EBS are explicitly accounted for in *Multiscale Thermohydrologic Model* (BSC 2004 [DIRS 163056]). This includes consideration of dryout near the waste packages, as well as evaporation or condensation within the drift and underneath the drip shield. The results of these analyses then feed *EBS Radionuclide Transport Abstraction* (BSC 2003 [DIRS 162728]).

As discussed in *In-Package Chemistry Abstraction* (BSC 2003 [DIRS 161962]), the thermal effects on the in-package chemistry are examined in the seepage drift model wherein EQ6 runs were performed at various temperatures to examine the temperature effect on the in-package chemistry. In these runs the kinetic reaction rates for the SNF were recalculated for runs at 15 to 90°C, and temperature-appropriate thermodynamic data in *In-Package Chemistry Abstraction* (BSC 2003 [DIRS 161962], Section 4.1.1.1) were used in the simulations.

For TSPA-LA the in-package chemistry abstractions of pH, ionic strength, total carbonate, and Eh are cast in terms of temperature (BSC 2003 [DIRS 161962], Sections 8.2.3, 8.2.6, 8.4.3, 8.4.6, 8.5, and 8.6; CRWMS M&O 2000 [DIRS 151561]), which captures the thermal effects on in-package chemistry.

### **Supporting Documents:**

BSC 2003 [DIRS 161962]

### **Related FEPs:**

- 2.1.08.04.0A, Condensation (Cold Traps) on Drift Roof
- 2.1.08.07.0A, Unsaturated Flow in EBS
- 2.1.08.14.0A, Condensation on Underside of Drip Shield
- 2.1.11.09.0A, Thermal Effects on Flow in EBS
- 2.1.11.03.0A, Exothermic Reactions in the EBS
- 2.1.12.04.0A, Gas Generation (CO<sub>2</sub>, CH<sub>4</sub>, H<sub>2</sub>S) From Microbial Degradation

## 6.2.35 Thermally Driven Flow (Convection) in the EBS

### **FEP Number:**

2.1.11.09.0B

**FEP Description**: Temperature differentials may result in convective flow in the EBS. Convective flow within the waste and EBS could influence in-package chemistry.

## **Descriptor Phrases:**

Thermally driven flow (convection) in-package

## **Screening Decision:**

Excluded (low consequence)

Screening Argument: Locally saturated conditions that could occur in a failed waste package containing liquid water could result in convective flow as a result of local thermal gradients. Such convective flow could serve to disperse corrosion by-products or dissolved radionuclides and result in an acceleration of those degradation processes. Thermally driven flow is not included in the TSPA-LA modeling, but its exclusion is conservative. The transport modeling as employed in *EBS Radionuclide Transport Abstraction* (BSC 2003 [DIRS 162728], Table 20 and Section 7.5.1) includes a single mixing cell in the waste package (Section 5.2.35 of this analysis report). Thermal convection inside the waste package would tend to erase concentration gradients and distribute radionuclides uniformly throughout the package. Also, the analysis of an alternative model for in-package chemistry (BSC 2003 [DIRS 161962], Section 6.4.1) treated the waste package as a one-dimensional assemblage of mixing cells with varying compositions. It was concluded therein that the single-mixing-cell primary (water vapor condensation) model was preferable because the effect of the materials within the waste package on the water chemistry overwhelmed the effect of any spatial variation due to temperature.

Furthermore, the breach of a waste package required for the admission of water is most likely to occur after 1000 years, by which time the temperature gradients are likely to be small (BSC 2004 [DIRS 165057], Appendix A).

Therefore, omission of convective flow within the waste package will not significantly change the radiological exposures to the reasonably maximally exposed individual and radionuclide releases to the accessible environment and this FEP can be excluded from the TSPA-LA based on low consequence.

## **TSPA Disposition:**

N/A

## **Supporting Documents:**

BSC 2003 [DIRS 161962] BSC 2003 [DIRS 162728] BSC 2004 [DIRS 165057]

### **Related FEPs:**

- 2.1.08.04.0A, Condensation (Cold Traps) on Drift Roof
- 2.1.08.07.0A, Unsaturated Flow in EBS
- 2.1.08.14.0A, Condensation on Underside of Drip Shield
- 2.1.11.09.0A, Thermal Effects on Flow in EBS
- 2.1.09.01.0B, Chemical Characteristics of Water in the Waste Package
- 2.1.09.01.0A, Chemical Interaction with Corrosion Products

## 6.2.36 Gas Generation (CO<sub>2</sub>, CH<sub>4</sub>, H<sub>2</sub>S) From Microbial Degradation

#### **FEP Number:**

2.1.12.04.0A

**FEP Description**: Microbes are known to produce inorganic acids, methane, organic byproducts, carbon dioxide, and other chemical species that could change the longevity of materials in the repository and the transport of radionuclides from the near field. The rate of microbial gas production will depend on the nature of the microbial populations established, the prevailing conditions (temperature, pressure, geochemical conditions), and the organic or inorganic substrates present. Initial analysis indicates the most important source of nutrient in the YMP repository will be metals. Other possible nutrients include cellulosic material, plastics, and synthetic materials. Minimal amounts of organics are mandated by regulation.

## **Descriptor Phrases:**

Internal gas pressure from CO<sub>2</sub>, CH<sub>4</sub>, H<sub>2</sub>S Gas accumulation under biofilms Chemical effects from CO<sub>2</sub>, CH<sub>4</sub>, H<sub>2</sub>S generation

### **Screening Decision:**

Excluded (low consequence)

Screening Argument: Gas generation from microbial degradation is excluded from TSPA-LA on the basis of low consequence. Omission of the effects of gas generation from microbial degradation on in-package waste chemistry will not significantly change radiological exposures to the reasonably maximally exposed individual or radionuclide releases to the environment for the following reasons. Generally speaking, the YMP system is considered to be an open system, and any gas produced will not accumulate in significant amounts to affect the system. Also, biological activity inside the waste package has been excluded (FEP 2.1.10.01.0A) because organic material will be present in only minor amounts in the waste package. Note also that methanogenesis and H<sub>2</sub>S generation are anaerobic processes. These will not occur under the oxidizing conditions that are expected to occur at Yucca Mountain. Finally, there may be some localized effects such as gas accumulation under biofilms. The possibility of local depression of pH by microbes is addressed in FEP 2.1.02.14.0A.

The sealed waste packages at emplacement will contain little oxygen or water, suggesting a low probability of gas generation from microbial degradation within the package. Once the package is breached, it may be reasonably concluded that any gas produced will migrate to the outside of the package. Gas produced from microbial degradation, because of the repository host rock

lithology and structure and physical properties of gas as it flows through these structures, will preferentially flow through stress-induced fractures and in situ fracture networks to eventually reach the mountain surface. Gas concentrations will become more dispersed and less concentrated as gas moves away from the repository; thus, gas concentrations become diluted before gas could accumulate in quantities of concern (see FEP 2.1.12.01.0A).

The primary potential impact of gas generation inside a breached waste package is likely to be associated with the generation of CO<sub>2</sub> by microorganisms. High levels of CO<sub>2</sub> might affect the in-package pH, as well as the solubilities of those radionuclides that complex appreciably with carbonate. Microbial respiration is potentially able to increase in-drift CO<sub>2</sub> production by two orders of magnitude (CRWMS M&O 2000 [DIRS 151561]). Absolute levels of carbon dioxide will depend not only on the production rate, but on the rate at which it leaves the drift as well. If diffusion of carbon dioxide is slow, high carbon dioxide levels might result (CRWMS M&O 2000 [DIRS 151561]). Sensitivity calculations in *In-Package Chemistry Abstraction* (BSC 2003 [DIRS 161962]) show that variations in carbon dioxide partial pressures from 10<sup>-4</sup> to 10<sup>-2</sup> have no effect on the outputs of the in-package chemistry model (10<sup>-3.5</sup> is the baseline atmospheric level of CO<sub>2</sub>). It is therefore reasonable to expect little impact of carbon dioxide production on in-package pH and ionic strength and to assume no impact from increased CO<sub>2</sub> levels.

Effects of carbon dioxide from microbial degradation on radioactive element solubilities will be small, as shown in the analysis of dissolved concentrations of radioactive elements in Finch and Fortner (2002 [DIRS 162004]), which encompassed carbon dioxide partial pressures as high as 1.0 to 1.5 atmospheres (see also Section 5.2.36 of this analysis report). *Dissolved Concentration Limits of Radioactive Elements* (BSC 2003 [DIRS 163152]) parameterizes for dissolved concentrations of radionuclides as a function of in-package and EBS solution chemistry over a range of carbon dioxide partial pressures of 10<sup>-5</sup> to 10<sup>-1.5</sup>—in effect to two orders of magnitude greater than atmospheric pressure. The CO<sub>2</sub> ranges, over which TSPA calculates probability distributions for radionuclide solubilities, bound high carbon dioxide levels. Therefore, any additional effects on radionuclide solubilities, from high carbon dioxide levels from microbial degradation would not be significant and can be excluded due to low consequence.

### **TSPA Disposition:**

N/A

## **Supporting Documents:**

BSC 2003 [DIRS 161962]

#### **Related FEPs:**

- 2.1.02.14.0A, Microbiologically Influenced Corrosion (MIC) of Cladding
- 2.1.10.01.0A, Microbial Activity in the EBS
- 2.1.12.01.0A, Gas generation (Repository Pressurization)

### 6.2.37 Effects of Radioactive Gases in EBS

### **FEP Number:**

2.1.12.07.0A

**FEP Description**: Radioactive gases may exist or be produced in the repository. These gases may subsequently escape from the repository. Typical radioactive gases include <sup>14</sup>C (in <sup>14</sup>CO<sub>2</sub> and <sup>14</sup>CH<sub>4</sub>) produced during microbial degradation, tritium, fission gases (Ar, Xe, Kr), and radon.

## **Descriptor Phrases:**

Gas generation in EBS
Gas exsolution in EBS
Repository pressurization
Effects of gas on waste package degradation

## **Screening Decision:**

Excluded (low consequence)

**Screening Argument**: The major gas constituents trapped inside a waste package prior to disposal will be the result of fission-product and neutron-activated stable and radioactive noble gases—predominantly isotopes of Ar, Kr, and Xe. There are several arguments that support the exclusion of radioactive gases from the TSPA-LA calculations, based on low consequence to waste package internal pressures and low consequence with respect to radionuclide releases from the EBS.

Radioactive gases residing in fuel rods and waste packages prior to postclosure or produced after postclosure times will either decay rapidly or quickly become negligible in terms of mass and volume. Specifically:

- A. Xenon (<sup>135</sup>Xe), a fission yield-product, is short-lived (9.2 hours) and will not be produced during the regulatory time periods. It will undergo decay to its long-lived daughter <sup>135</sup>Cs by the time of waste emplacement.
- B. Argon (<sup>39</sup>Ar) has a low activity and is screened out due to low consequence. It will not be produced during the regulatory time period.
- C. Radon gas (<sup>222</sup>Rn and <sup>219</sup>Rn) is short-lived (approximately 3.8 days and approximately 4 seconds, respectively), as are its gaseous daughters (<sup>218</sup>Po, half-life approximately 3.1 minutes and <sup>215</sup>Po, half-life of microseconds) and, thus, will be in secular equilibrium with its parents, radium and thorium (<sup>229</sup>Th). Radon has been screened out of the TSPA-LA due to low consequence.
- D. <sup>14</sup>CH<sub>4</sub> and <sup>14</sup>CO<sub>2</sub> generation from microbial activity (CRWMS M&O 2000 [DIRS 151561], Sections 6.3 and 7.2) should not be significant because organic levels in the waste are expected to be low.
- E. Once a waste package is breached, an oxidizing environment may be created within the waste package, thus enabling <sup>14</sup>CO<sub>2</sub> to be formed. The limited amount of <sup>14</sup>C remaining in the inventory, coupled with the low package-failure rate, limits the potential creation of <sup>14</sup>CO<sub>2</sub> to small amounts. Furthermore, the amounts of <sup>14</sup>C transported as a gas to the accessible environment will be extremely small, so the risk

consequence is negligible. See FEP 2.2.11.03.0A in *Features, Events, and Processes in UZ Flow and Transport* (BSC 2004 [DIRS 168782], Section 6.1.39).

F. Of the noble gases, <sup>85</sup>Kr has a significant initial inventory, but because of its short half-life (approximately 10 years), its concentration rapidly becomes insignificant.

Partial pressures from radioactive gas will not be great enough to compromise waste package integrity via a waste package breach (BSC 2004 [DIRS 162200], Section 6.2.13.5). This argument is supported by several numerical studies investigating the sensitivity of internal waste package pressures presuming fuel rods rupture, thus causing a release of gases from the fuel matrix to the waste package interior (CRWMS M&O 1997 [DIRS 100264]; CRWMS M&O 2000 [DIRS 144128]; BSC 2001 [DIRS 153755]). These studies conservatively estimate that the maximum pressures within the fuel-rod cladding would rise to 8.4 MPa (CRWMS M&O 1997 [DIRS 100264], Section 7.2.2.7), thus inducing clad failure. Once cladding ruptured, all radioactive and fission gases migrated from the fuel matrix to the waste package voids. Waste package interior pressures were determined for cases presuming 1, 10, and 100 percent of all fuel rods rupture (CRWMS M&O 1997 [DIRS 100264], Table 7.2.2.7-1), and rupture occurs at temperatures ranging from 20 to 600°C. An additional case presumes all fuel rods rupture, and all fuel pellets have a 50-percent higher burnup. Consequently, internal pressures would be greater than assemblies experiencing normal burnup conditions by a factor of 1.5 (CRWMS M&O 1997 [DIRS 100264], Section 7.2.2.7). Analyses of stresses imposed on the waste package interior shells by internal pressurization resulting from fuel rod rupture (CRWMS M&O 2000 [DIRS 144128], Table 21) determined the maximum allowable waste package interior pressures for various waste package designs (BSC 2001 [DIRS 153755], Table 6-1).

Results from these studies show that even assuming 100 percent fuel rod failure, expected interior waste package pressures for normal burnup rates (CRWMS M&O 1997 [DIRS 100264], Table 7.2.2.7-1) are consistently and significantly lower than the maximum allowable for the various waste package loadings (CRWMS M&O 1997 [DIRS 100264], Table 7.2.2.7-1). For example, in the high burnup cases (using the 1.5 multiplier), the waste package pressure at 200°C is 0.62 MPa, much lower than the pressure of 1.02 to 1.81 MPa required to cause the waste package outer shell to fail (BSC 2001 [DIRS 153755], Table 6-1). The above studies are upper-limit bounded for several reasons. It is estimated that nominal waste package temperatures for the base case will not exceed 350°C, well below the 500°C used in the analysis performed in Waste Package Design Basis Events (CRWMS M&O 1997 [DIRS 100264]). Not all the fuel rods will rupture within a waste package within the regulatory time frame. Furthermore, fission and radioactive gas release fractions from the fuel matrix are typically low (CRWMS M&O 2000 [DIRS 151659], Section 6.3.3). Therefore, fission gas released from the matrix will not all migrate to 'free' void space, especially at temperatures approaching 27°C, where migration of fission gases, including radioactive gases, out of the matrix approaches 0.0 (CRWMS M&O 1997 [DIRS 100264]). This FEP may therefore be screened as excluded due to low consequence.

### **TSPA Disposition:**

N/A

### Supporting Documents:

CRWMS M&O 2000 [DIRS 144128] CRWMS M&O 2000 [DIRS 151659] BSC 2001 [DIRS 153755]

#### **Related FEPs:**

N/A

### 6.2.38 Radiolysis

#### **FEP Number:**

2.1.13.01.0A

**FEP Description**: Alpha, beta, gamma, and neutron irradiation of water can cause disassociation of molecules, leading to gas production and changes in chemical conditions (Eh, pH, concentration of reactive radicals).

# **Descriptor Phrases:**

Gas generation from radiolysis Chemical effects from radiolysis in-package

## **Screening Decision:**

Excluded (low consequence)

Screening Argument: The effects of radiolysis for gas production and waste form chemistry can be excluded from consideration in the TSPA based on low consequence. Alpha, beta, gamma, and neutron irradiation of water leads to formation of highly reactive excited and ionized species. In pure water, the final products are hydrogen and oxidants. In addition, the oxidants formed may react with dissolved iron (+2) which will decrease the net yield of oxidants. However, water is not expected to affect the fuel until all, except possibly alpha radiolysis, have become significantly reduced. The effects of beta irradiation are expected to be minimal because 1) almost all beta emitters disappear due to radioactive decay after a few hundred years and 2) beta radiation is stopped in the fuel matrix or clad. Recent calculations by Tang have shown that neutron irradiation is negligible and gamma dose has been significantly reduced (BSC 2002 [DIRS 161912]). Intact cladding will stop alpha particles so alpha radiolysis will not occur during the early periods of highest alpha activity. Additionally, the rate of corrosion effects of used UO<sub>2</sub> fuel due to alpha radiolysis, taking no credit for cladding, can be predicted (based on semiempirical methods) to have low consequence.

Interior to the waste package, water will not intrude (i.e., the waste container will not fail) until gamma and beta emitters have decayed to low concentrations (Sunder and Shoesmith 1991 [DIRS 143815]; Shoesmith and Sunder 1992 [DIRS 113368]). According to Sunder and Shoesmith (1991 [DIRS 143815]), "strong gamma and beta fields associated with the used fuel will decrease by a factor greater than 10<sup>3</sup> in the first few hundred years after disposal...." Arguments addressing the highly improbable adverse or inconsequential impact of nitric acid and hydrogen peroxide production, and other potential products, of gamma radiolysis on corrosion are presented in *In-Package Chemistry for Waste Forms* (BSC 2003 [DIRS 168795], Attachment II) and *In-Package Chemistry Abstraction* (BSC 2003 [DIRS 161962]). In this

analysis, the production of nitric acid and hydrogen peroxide was increased by a factor of ten. The effect of in-package chemistry was to change the chemical compositions in the second significant figure; however, this effect is insignificant.

The use of presently available used fuels to study the effects of alpha radiolysis on fuel dissolution is inappropriate because of their associated strong beta and gamma fields. However, Sunder et al. (1997 [DIRS 143860]) describe an experimental strategy for determining fuel dissolution rates as a function of alpha-source strength, and they show how the evolution of corrosion behavior can be predicted as a function of the age of the fuel. Sunder et al. (1997 [DIRS 143860]) conclude that "predictions presented…suggest the effects of alpha radiolysis on fuel corrosion (dissolution) will be transitory and will become minor as alpha dose rates decrease."

During the periods of highest alpha activity, it is expected most of the commercial fuel cladding will remain intact and should substantially reduce alpha dose rates to groundwater (Kaplan 1963 [DIRS 149367], p. 307). The stopping power of metals is at least three orders of magnitude greater than air; thus clad of thickness of a few microns would stop alpha particles.

Additionally, there are these two net findings:

- 1. The  $\alpha$ -radiolysis-enhanced corrosion rate is three orders of magnitude less than the dissolution rate.
- 2. The  $\alpha$ -radiolysis-enhanced corrosion rates for HLW metallic carbide, and ceramic spent nuclear fuels are much lower than their dissolution rates.

Since no credit is being taken for the DSNF cladding in the TSPA, the effect of radiolysis on the DSNF cladding is not a factor. However, the argument by Sunder et al. (1997 [DIRS 143860]) does not include the protection of clad against dissolution.

This FEP does not have a significant effect on radiological exposures to the reasonably maximally exposed individual and radionuclide releases to the accessible environment and may therefore be screened as excluded due to low consequence.

### **TSPA Disposition:**

N/A

### **Supporting Documents:**

BSC 2003 [DIRS 168795] BSC 2003 [DIRS 161962]

#### **Related FEPs:**

2.1.13.02.0A

### **6.2.39 Radiation Damage in EBS**

#### **FEP Number:**

2.1.13.02.0A

**FEP Description**: Radiolysis due to the alpha, beta, gamma ray, and neutron irradiation of water could result in the enhancement for the movement of the radionuclides from the surface of a degraded waste form into groundwater flow. When radionuclides decay, the emitted highenergy particle could result in the production of radicals in the water or air surrounding the spent nuclear fuel. If these radicals migrate (diffuse) to the surface of the fuel, they may then enhance the degradation/corrosion rate of the fuel (UO<sub>2</sub>). This effect would increase the dissolution rate for radionuclides from the fuel material (fuel meat) into the groundwater flow. Strong radiation fields could lead to radiation damage to the waste forms and containers (CSNF, DSNF, and DHLW), drip shield, seals and surrounding rock.

# **Descriptor Phrases:**

Enhanced waste form degradation from radiation Radiation damage in-package (waste form)

## **Screening Decision:**

Excluded (low consequence)

Screening Argument: Radiation damage can be caused by low linear energy transfer (i.e., beta particles and gamma rays) and high linear energy transfer (i.e., alpha) radiation. Low linear energy transfer radiation (mostly gamma rays) effects are relatively reduced (in comparison to high linear energy transfer effects) because the radiation fields decrease dramatically over the first 1,000 years after the fuel is outside the reactor (Sunder et al. 1997 [DIRS 143860], p. 67). The effect of high linear energy transfer radiation on fuel degradation will depend on the time at which cladding integrity is lost for a given fuel rod (the high linear energy transfer radiation would not be able to penetrate past the cladding material while intact cladding material is present). Before the cladding is significantly compromised (by cracking, pitting, unzipping, etc.), the damage due to radiolysis will be dominated by low linear energy transfer radiation. After cladding material is lost, the radiolysis rate will be dominated by high linear energy transfer radiation. High linear energy transfer alpha radiation fields will persist for tens of thousands of years.

Of the various modes of radioactive decay (i.e., alpha [ $\alpha$ -], beta [ $\beta$ -], gamma [ $\gamma$ -], spontaneous fission, isomeric transition, etc.), the most important for fissile materials (Attachment IV of this analysis report) is  $\alpha$ -decay. Radionuclides that decay by other modes have correspondingly relatively short half-lives (i.e., tens to hundreds of years); thus, they would decay away prior to the estimated time to corrosion breakthrough of the fuel cladding. The dominant decay mode for heavy radionuclides is  $\alpha$ -decay. While many of the heavy radionuclides emit alpha particles with energies greater than 4.0 MeV (Parrington et al. 1996 [DIRS 103896]), there are no gamma releases or beta particles emitted with energies greater than 4.0 MeV and only a few with energies greater than 1.0 MeV. Thus,  $\alpha$ -decay linear energy transfer values will bound the effects due to beta particles and gamma rays. Also the majority of the long-term radionuclides for YMP are alpha emitters. Other special decay modes such as isomeric transition and spontaneous fission decay have probabilities of occurrence that are orders of magnitude less than that for alpha decay.

Radioactive decay of radionuclides after they have entered the groundwater is not of concern since they will not, to any measurable quantity, increase the release of radionuclides from the

waste forms into the groundwater. The decay within the groundwater will only transmute the specific radionuclide inventory already being transported by the groundwater (i.e., due to colloids, dissolution, etc.), and the subsequent decay chains from the transported radionuclides should be modeled within the radionuclide transport computational codes.

This FEP does not have a significant effect on radiological exposures to the reasonably maximally exposed individual and radionuclide releases to the accessible environment and may therefore be screened as excluded due to low consequence. Related processes of alpha recoil (see FEP 2.1.02.04.0A) and radiolysis (see FEP 2.1.13.01.0A) are also excluded based on low consequence.

## **TSPA Disposition:**

N/A

### **Supporting Documents:**

N/A

#### **Related FEPs:**

- 2.1.12.03.0A, Gas Generation (H<sub>2</sub>) From Metal Corrosion
- 2.1.02.04.0A, Alpha Recoil Enhances Dissolution
- 2.1.13.01.0A, Radiolysis
- 3.1.01.01.0A, Radioactive Decay and In-Growth

## 6.2.40 Chemistry of Water Flowing into Waste Package

### **FEP Number:**

2.2.08.12.0B

**FEP Description**: Inflowing water chemistry may be used in analysis or modeling that requires initial water chemistry in the waste package.

### **Descriptor Phrases:**

Inflowing water composition (into waste package)

### **Screening Decision:**

Included

## **Screening Argument:**

N/A

**TSPA Disposition**: Three different initial water compositions were used to represent the chemistry of the water flowing into the waste package. This inflowing water chemistry is one of the inputs used to determine the in-package chemistry in the IPCM. Therefore, the variability of the incoming water composition is implicitly included in the in-package chemistry and in the abstractions passed to TSPA in *In-Package Chemistry Abstraction* (BSC 2003 [DIRS 161962]). In TSPA it then feeds the solubility, colloid, CSNF, and HLW glass submodels. The effects of the inflowing water chemistry are captured within the IPCM parameters: pH, ionic strength, total carbonate, Eh, chloride, and fluoride.

The seepage dripping model examined various input water chemistries (BSC 2003 [DIRS 161962], Section 4.1.1.2) and their effect on the in-package chemistry. The results showed the parameters passed to TSPA-LA were unaffected by changes in the input water composition. Thus, while the composition of the water flowing into the waste package is implicitly included in the TSPA-LA model, variations in the composition do not significantly affect the model results.

### **Supporting Documents:**

BSC 2003 [DIRS 161962]. (Note that while FEP 2.2.08.12.0B is not in the included FEP table (BSC 2003 [DIRS 161962], Table 10), it is addressed in the report.)

### **Related FEPs:**

2.1.09.01B, Chemical characteristics of water in the waste package

### 6.2.41 Radioactive Decay and In-growth

### **FEP Number:**

3.1.01.01.0A

**FEP Description**: Radioactivity is the spontaneous disintegration of an unstable atomic nucleus that results in the emission of subatomic particles. Radioactive isotopes are known as radionuclides. Radioactive decay of the fuel in the repository changes the radionuclide content in the fuel with time and generates heat. Radionuclide quantities in the system at any time are the result of the radioactive decay and the growth of daughter products as a consequence of that decay (i.e., ingrowth). Over a 10,000-year performance period, these processes will produce daughter products that need to be considered in order to adequately evaluate the release and transport of radionuclides to the accessible environment.

### **Descriptor Phrases:**

Radioactive decay and ingrowth (in package) Radioactive decay and ingrowth (in drift)

### **Screening Decision:**

Included

### **Screening Argument:**

N/A

**TSPA Disposition**: Radioactive decay and in-growth were considered in the selection of isotopes of importance to TSPA-LA and are included as standard features of the GoldSim code. Once the isotopes most important to dose were identified (BSC 2002 [DIRS 160059], Table 13), the parents of these isotopes were examined to determine if decay and in-growth could significantly affect the amount of the important isotopes during the regulatory period. Seven parent isotopes were identified whose decay significantly increased the amount of their progeny (BSC 2003 [DIRS 161961], Table 16):

$$\bullet \overset{245}{\text{Cm}} \rightarrow \overset{241}{\text{Pu}} \rightarrow \overset{241}{\text{Am}}$$

$$\bullet \overset{235}{\text{U}} \rightarrow \overset{231}{\text{Pa}}$$

- $^{230}$ Th  $\rightarrow$   $^{226}$ Ra
- $^{232}$ Th  $\rightarrow$   $^{228}$ Ra
- $^{236}U \rightarrow ^{232}Th$
- $^{242}$ Pu  $\rightarrow$   $^{238}$ U

These seven isotopes were added to the list of isotopes to be tracked in the TSPA-LA GoldSim model. During execution, the GoldSim model automatically calculates decay and in-growth of the included isotopes within the waste package and drift modeling cells.

## **Supporting Documents:**

BSC 2003 [DIRS 161961]

### **Related FEPs:**

2.1.01.01.0A, Waste inventory

Miscellaneous Waste-Form FEPs

INTENTIONALLY LEFT BLANK

#### 7. CONCLUSIONS

This scientific analysis report addresses 41 waste form and waste form colloid FEPs. These FEPs were identified and examined for inclusion or exclusion in TSPA-LA. Table 1.2-1 lists these FEPs and their associated screening decisions.

By default, a FEP is included in the TSPA if it cannot be excluded based on the screening criteria described in Section 4.2.1. For included FEPs, the TSPA-LA Dispositions provided in Section 6.2 describe how each FEP is included in the TSPA-LA (i.e., through a parameter or TSPA model or sub-model). For excluded FEPs, the screening decision is based on the screening criteria (by regulation, low probability, or low consequence) and the technical basis for exclusion is elaborated in the screening arguments provided in Section 6.2.

The analyses developed in this report are qualitative, based on available project information and the open technical literature, and so any uncertainties associated with the FEPs screening decisions are also qualitative.

The following conclusions may be drawn:

- This analysis model report contributes to Yucca Mountain FEP analysis by screening 41 miscellaneous WF FEPs. This report extracts the TSPA-disposition statements for included FEPs from the pertinent model reports and presents the screening arguments for excluded FEPs. This analysis model report provides both information for the YMP FEP database and guidance to TSPA analyses.
- By providing references to appropriate other analysis model reports, this report provides a link between WF issues and the research directed at their resolution.

Miscellaneous Waste-Form FEPs

INTENTIONALLY LEFT BLANK

#### 8. INPUTS AND REFERENCES

### 8.1 DOCUMENTS CITED

- Abrefah, J.; Gray, W.J.; Ketner, G.L.; Marschman, S.C.; Pyecha, T.D.; and Thornton, T.A. 1995. *K-Basin Spent Nuclear Fuel Characterization Data Report*. PNL-10778. Richland, Washington: Pacific Northwest National Laboratory. TIC: 243197.
- Abrefah, J.; Huang, F.H.; Gerry, W.M.; Gray, W.J.; Marschman, S.C.; and Thornton, T.A. 1999. *Analysis of Ignition Testing on K-West Basin Fuel*. PNNL-11816. Richland, Washington: Pacific Northwest National Laboratory. TIC: 248558.
- Adkins, H.E. 2003. "Transmittal of Draft Version of Validation of Dissolved Concentrations, Argonne National Laboratory." Interoffice memorandum from H.E. Adkins (BSC) to Y. Chen, June 19, 2003, 0617037708, with attachment. ACC: MOL.20030619.0100. TBV-5177
- Bruno, J.; Cera, E.; Eklund, U.-B.; Eriksen, T.E.; and Grive, M. 1998. *Some Preliminary Modeling Results of Long Term Radiolytic Mass Balance Experiments*. Presentation at the Spent Fuel Workshop 1998, Las Vegas, Nevada, May 18-20, 1998. Barcelona, Spain: Quantisci. TIC: 240716.
- BSC (Bechtel SAIC Company) 2001. *In-Drift Microbial Communities Model Validation Calculations*. CAL-EBS-EV-000001 REV 00 ICN 02. Las Vegas, Nevada: Bechtel SAIC Company. ACC: MOL.20020107.0156.
- 153755 BSC 2001. *Internal Pressurization Due to Fuel Rod Rupture in Waste Packages*. CAL-EBS-ME-000005 REV 01. Las Vegas, Nevada: Bechtel SAIC Company. ACC: MOL.20010629.0076.
- 154365 BSC 2001. *The Development of Information Catalogued in REV00 of the YMP FEP Database*. TDR-WIS-MD-000003 REV 00 ICN 01. Las Vegas, Nevada: Bechtel SAIC Company. ACC: MOL.20010301.0237.
- BSC 2002. Gamma and Neutron Radiolysis in the 21-PWR Waste Package from Ten to One Million Years. 000-00C-DSU0-00700-000-00A. Las Vegas, Nevada: Bechtel SAIC Company. ACC: MOL.20021004.0002.
- 160059 BSC 2002. *Radionuclide Screening*. ANL-WIS-MD-000006 REV 01. Las Vegas, Nevada: Bechtel SAIC Company. ACC: MOL.20020923.0177.
- 160313 BSC 2002. *Scientific Processes Guidelines Manual*. MIS-WIS-MD-000001 REV 01. Las Vegas, Nevada: Bechtel SAIC Company. ACC: MOL.20020923.0176.
- BSC 2002. The Enhanced Plan for Features, Events, and Processes (FEPs) at Yucca Mountain. TDR-WIS-PA-000005 REV 00. Las Vegas, Nevada: Bechtel SAIC Company. ACC: MOL.20020417.0385.

- BSC 2003. *Dike/Drift Interactions*. MDL-MGR-GS-000005 REV 00. Las Vegas, Nevada: Bechtel SAIC Company. ACC: DOC.20031022.0001.
- BSC 2003. Dissolved Concentration Limits of Radioactive Elements. ANL-WIS-MD-000010 REV 02. Las Vegas, Nevada: Bechtel SAIC Company. ACC: DOC.20030624.0003.
- BSC 2003. DSNF and Other Waste Form Degradation Abstraction. ANL-WIS-MD-000004 REV 02. Las Vegas, Nevada: Bechtel SAIC Company. ACC: DOC.20030711.0002.
- BSC 2003. *In-Package Chemistry for Waste Forms*. ANL-EBS-MD-000056 REV 00, with errata. Las Vegas, Nevada: Bechtel SAIC Company. ACC: MOL.20010322.0490; DOC.20031014.0005.
- BSC 2003. Risk Information to Support Prioritization of Performance Assessment Models. TDR-WIS-PA-000009 REV 01 ICN 01, with errata. Las Vegas, Nevada: Bechtel SAIC Company. ACC: MOL.20021017.0045; DOC.20031014.0003.
- BSC 2003. *In-Package Chemistry Abstraction*. ANL-EBS-MD-000037 REV 02. Las Vegas, Nevada: Bechtel SAIC Company. ACC: DOC.20030723.0003.
- BSC 2003. *Initial Radionuclide Inventories*. ANL-WIS-MD-000020 REV 00. Las Vegas, Nevada: Bechtel SAIC Company. ACC: DOC.20031110.0002.
- 165179 BSC 2003. *Q-List*. TDR-MGR-RL-000005 REV 00. Las Vegas, Nevada: Bechtel SAIC Company. ACC: DOC.20030930.0002.
- BSC 2003. *Total System Performance Assessment-License Application Methods and Approach*. TDR-WIS-PA-000006 REV 00 ICN 01. Las Vegas, Nevada: Bechtel SAIC Company. ACC: DOC.20031215.0001.
- BSC 2003. Waste Form and In-Drift Colloids-Associated Radionuclide
  Concentrations: Abstraction and Summary. MDL-EBS-PA-000004 REV 00 ICN 01.
  Las Vegas, Nevada: Bechtel SAIC Company. ACC: DOC.20031222.0012.
- BSC 2004. *Clad Degradation FEPs Screening Arguments*. ANL-WIS-MD-000008 REV 01. Las Vegas, Nevada: Bechtel SAIC Company. ACC: DOC.20040322.0001.
- BSC 2004. *CSNF Waste Form Degradation: Summary Abstraction*. ANL-EBS-MD-000015 REV 01, with errata. Las Vegas, Nevada: Bechtel SAIC Company. ACC: DOC.20030708.0004; DOC.20031224.0001; DOC.20040202.0002.
- 167619 BSC 2004. *Defense HLW Glass Degradation Model*. ANL-EBS-MD-000016 REV 01 ICN 01. Las Vegas, Nevada: Bechtel SAIC Company. ACC: DOC.20040223.0006.

- BSC 2004. EBS Radionuclide Transport Abstraction, Check Copy 3/15/2004. ANL-WIS-PA-000001 REV 01. Las Vegas, Nevada: Bechtel SAIC Company. ACC: MOL.20040414.0096. TBV-5787
- 167461 BSC 2004. Engineered Barrier System: Physical and Chemical Environment Model. ANL-EBS-MD-000033 REV 02. Las Vegas, Nevada: Bechtel SAIC Company. ACC: DOC.20040212.0004.
- BSC 2004. Features, Events, and Processes in UZ Flow and Transport. ANL-NBS-MD-000001 REV 02. Las Vegas, Nevada: Bechtel SAIC Company. ACC: DOC.20040331.0002.
- BSC 2004. FEPs Screening of Processes and Issues in Drip Shield and Waste Package Degradation. ANL-EBS-PA-000002 REV 02. Las Vegas, Nevada: Bechtel SAIC Company. ACC: DOC.20040408.0001.
- BSC 2004. *Igneous Intrusion Impacts on Waste Packages and Waste Forms*. MDL-EBS-GS-000002 REV 01D. Las Vegas, Nevada: Bechtel SAIC Company. ACC: MOL.20040414.0095. TBV-5788
- BSC 2004. *Multiscale Thermohydrologic Model*. ANL-EBS-MD-000049 REV 01. Las Vegas, Nevada: Bechtel SAIC Company. ACC: DOC.20040301.0004.
- BSC 2004. Technical Work Plan for Waste Form Degradation Modeling, Testing, and Analyses in Support of LA. TWP-WIS-MD-000008 REV 02 ICN 04. Las Vegas, Nevada: Bechtel SAIC Company. ACC: DOC.20040218.0001.
- BSC 2004. Technical Work Plan for: Decision Support and Documentation Department Activities. TWP-MGR-MD-000028 REV 04. Las Vegas, Nevada: Bechtel SAIC Company. ACC: DOC.20040303.0003.
- Buck, E.C.; Finch, R.J.; Finn, P.A.; and Bates, J.K. 1998. "Retention of Neptunium in Uranyl Alteration Phases Formed During Spent Fuel Corrosion." *Scientific Basis for Nuclear Waste Management XXI, Symposium held September 28-October 3, 1997, Davos, Switzerland.* McKinley, I.G. and McCombie, C., eds. 506, 87-94. Warrendale, Pennsylvania: Materials Research Society. TIC: 240702.
- Buck, E.C.; McNamara, B.K.; Douglas, M.; and Hanson, B.D. 2003. *Possible Incorporation of Neptunium in Uranyl (VI) Alteration Phases*. PNNL-14277. Richland, Washington: Pacific Northwest National Laboratory. ACC: MOL.20040202.0085.
- Burns, P.C.; Ewing, R.C.; and Miller, M.L. 1997. "Incorporation Mechanisms of Actinide Elements into the Structures of U<sup>6+</sup> Phases Formed During the Oxidation of Spent Nuclear Fuel." *Journal of Nuclear Materials*, 245, (1), 1-9. Amsterdam, The Netherlands: North-Holland. TIC: 235501.

- 166275 Canori, G.F. and Leitner, M.M. 2003. *Project Requirements Document*. TER-MGR-MD-000001 REV 02. Las Vegas, Nevada: Bechtel SAIC Company. ACC: DOC.20031222.0006.
- 161997 Chen, Y. 2001. "An Empirical Np Solubility Model Based on Spent Fuel Dissolution Experiments." "Back to the Future Managing the Back End of the Nuclear Fuel Cycle to Create a More Secure Energy Future," Proceedings of the 9th International High-Level Radioactive Waste Management Conference (IHLRWM), Las Vegas, Nevada, April 29-May 3, 2001. La Grange Park, Illinois: American Nuclear Society. TIC: 247873.
- 162709 Chen, Y. 2003. "Using Reactive Transport Modeling to Evaluate the Source Term at Yucca Mountain." *Computers & Geosciences*, 29, (3), 385-397. New York, New York: Pergamon. TIC: 254363.
- Chen, Y.; Loch, A.R.; Wolery, T.J.; Steinborn, T.L.; Brady, P.V.; and Stockman, C.T. 2002. "Solubility Evaluation for Yucca Mountain TSPA-SR." *Scientific Basis for Nuclear Waste Management XXV, Symposium held November 26-29, 2001, Boston, Massachusetts*. McGrail, B.P. and Cragnolino, G.A., eds. 713, 775-782. Warrendale, Pennsylvania: Materials Research Society. TIC: 248663.
- Chen, Y.; Siegmann, E.; Mattie, P.; NcNeish, J.; Sevougian, S.D.; and Andrews, R. 1999. "A Mechanistic Model of Spent Fuel Dissolution, Secondary Mineral Precipitation, and Np Release." *Scientific Basis for Nuclear Waste Management XXII, Symposium held November 30-December 4, 1998, Boston, Massachusetts, U.S.A.* Wronkiewicz, D.J. and Lee, J.H., eds. 556, 471-478. Warrendale, Pennsylvania: Materials Research Society. TIC: 246426.
- 101234 Cranwell, R.M.; Guzowski, R.V.; Campbell, J.E.; and Ortiz, N.R. 1990. *Risk Methodology for Geologic Disposal of Radioactive Waste, Scenario Selection Procedure*. NUREG/CR-1667. Washington, D.C.: U.S. Nuclear Regulatory Commission. ACC: NNA.19900611.0073.
- 142613 Croff, A.G. 1980. *A User's Manual for the ORIGEN2 Computer Code*. ORNL/TM-7175. Oak Ridge, Tennessee: Oak Ridge National Laboratory. TIC: 225504.
- 101554 Croff, A.G. 1980. *ORIGEN2 A Revised and Updated Version of the Oak Ridge Isotope Generation and Depletion Code*. ORNL-5621. Oak Ridge, Tennessee: Oak Ridge National Laboratory. ACC: NNA.19910326.0094.
- 100264 CRWMS M&O 1997. *Waste Package Design Basis Events*. BBA000000-01717-0200-00037 REV 00. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19971006.0075.
- 100362 CRWMS M&O 1998. "Waste Form Degradation, Radionuclide Mobilization, and Transport Through the Engineered Barrier System." Chapter 6 of *Total System Performance Assessment-Viability Assessment (TSPA-VA) Analyses Technical Basis*

- *Document*. B00000000-01717-4301-00006 REV 01. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19981008.0006.
- 105649 CRWMS M&O 1998. *Immobilized in Ceramic*. Volume II of *Report on Intact and Degraded Criticality for Selected Plutonium Waste Forms in a Geologic Repository*. BBA000000-01717-5705-00020 REV 01. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19981217.0112.
- 100374 CRWMS M&O 1998. Waste Form Degradation and Radionuclide Mobilization Expert Elicitation Project. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19980804.0099.
- 136428 CRWMS M&O 1999. *BWR Source Term Generation and Evaluation*. BBAC00000-01717-0210-00006 REV 01. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.20000113.0334.
- 103955 CRWMS M&O 1999. *License Application Design Selection Report*. B00000000-01717-4600-00123 REV 01. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19990528.0303.
- 136429 CRWMS M&O 1999. *PWR Source Term Generation and Evaluation*. BBAC00000-01717-0210-00010 REV 01. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.20000113.0333.
- 144128 CRWMS M&O 2000. Design Analysis for UCF Waste Packages. ANL-UDC-MD-000001 REV 00. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.20000526.0336.
- 147651 CRWMS M&O 2000. Evaluation of Codisposal Viability for HEU Oxide (Shippingport PWR) DOE-Owned Fuel. TDR-EDC-NU-000003 REV 00. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.20000227.0240.
- 147650 CRWMS M&O 2000. Evaluation of Codisposal Viability for UZrH (TRIGA) DOE-Owned Fuel. TDR-EDC-NU-000001 REV 00. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.20000207.0689.
- 151561 CRWMS M&O 2000. *In-Drift Microbial Communities*. ANL-EBS-MD-000038 REV 00 ICN 01. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.20001213.0066.
- 151659 CRWMS M&O 2000. *Initial Cladding Condition*. ANL-EBS-MD-000048 REV 00 ICN 01. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.20001002.0145.
- 153595 CRWMS M&O 2000. Relative Contribution of Individual Radionuclides to Inhalation and Ingestion Dose. CAL-WIS-MD-000002 REV 00. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.20010103.0211.

- 153246 CRWMS M&O 2000. Total System Performance Assessment for the Site Recommendation. TDR-WIS-PA-000001 REV 00 ICN 01. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.20001220.0045.
- 151940 CRWMS M&O 2000. Unsaturated Zone Flow and Transport Model Process Model Report. TDR-NBS-HS-000002 REV 00 ICN 02. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.20000831.0280.
- DOE (U.S. Department of Energy) 1997. *EM/RW Repository Task Team Report:* Grouping Method to Minimize Testing for Repository Emplacement of DOE SNF. DOE/SNF/REP-008, Rev. 0. Idaho Falls, Idaho: U.S. Department of Energy. TIC: 247664.
- DOE 1998. *Total System Performance Assessment*. Volume 3 of *Viability Assessment of a Repository at Yucca Mountain*. DOE/RW-0508. Washington, D.C.: U.S. Department of Energy, Office of Civilian Radioactive Waste Management. ACC: MOL.19981007.0030.
- 122980 DOE 1998. Update to Assessment of Direct Disposal in Unsaturated Tuff of Spent Nuclear Fuel and High-Level Waste Owned by U.S. Department of Energy. DOE/SNF/REP-015. Washington, D.C.: U.S. Department of Energy. TIC: 243859.
- 118968 DOE 2000. *DOE Spent Nuclear Fuel Grouping in Support of Criticality, DBE, TSPA-LA*. DOE/SNF/REP-0046, Rev. 0. Idaho Falls, Idaho: U.S. Department of Energy, Idaho Operations Office. ACC: DOC.20030905.0021.
- DOE 2002. *DOE Spent Nuclear Fuel Information in Support of TSPA-SR*. DOE/SNF/REP-047, Rev. 2. Idaho Falls, Idaho: U.S. Department of Energy, Idaho Operations Office. TIC: 252089.
- DOE 2002. Waste Acceptance System Requirements Document. DOE/RW-0351, Rev. 4. Washington, D.C.: U.S. Department of Energy, Office of Civilian Radioactive Waste Management. ACC: MOL.20020326.0056.
- DOE 2002. Yucca Mountain Science and Engineering Report. DOE/RW-0539, Rev.
   Washington, D.C.: U.S. Department of Energy, Office of Civilian Radioactive Waste Management. ACC: MOL.20020404.0042.
- DOE 2004. *Quality Assurance Requirements and Description*. DOE/RW-0333P, Rev. 14. Washington, D.C.: U.S. Department of Energy, Office of Civilian Radioactive Waste Management. ACC: DOC.20040331.0004.
- Finch, R.J. and Fortner, J.A. 2002. *Dissolved Concentration Limits: Neptunium in Alteration Phases, A Progress Report.* Argonne, Illinois: Argonne National Laboratory. ACC: MOL.20031119.0180.
- Finch, R.J.; Fortner, J.A.; Buck, E.C.; and Wolf, S.F. 2002. "Neptunium Incorporation into Uranium(VI) Compounds Formed During Aqueous Corrosion of

- Neptunium-Bearing Uranium Oxides." *Scientific Basis for Nuclear Waste Management XXV, Symposium held November 26-29, 2001, Boston, Massachusetts.* McGrail, B.P. and Cragnolino, G.A., eds. 713, 647-654. Warrendale, Pennsylvania: Materials Research Society. TIC: 248663.
- Foster, A.R. and Wright, R.L., Jr. 1973. *Basic Nuclear Engineering*. 2nd Edition. Boston, Massachusetts: Allyn and Bacon. TIC: 247586.
- 165394 Freeze, G. 2003. *KTI Letter Report, Response to Additional Information Needs on TSPAI 2.05 and TSPAI 2.06*. REG-WIS-PA-000003 REV 00 ICN 04. Las Vegas, Nevada: Bechtel SAIC Company. ACC: DOC.20030825.0003.
- Friese, J.I. 2003. "Transmittal of Draft Version of Existing Evidence for the Fate of Neptunium in the Yucca Mountain Repository, Pacific Northwest National Laboratory." Interoffice memorandum from J.I. Friese (BSC) to Y. Chen, June 17, 2003, 0613037658, with attachment. ACC: MOL.20030617.0128. TBV-5174
- Friese, J.I.; Buck, E.C.; McNamara, B.K.; Hanson, B.D.; and Marschman, S.C. 2003. *Existing Evidence for the Fate of Neptunium in the Yucca Mountain Repository*. PNNL-14307. Richland, Washington: Pacific Northwest National Laboratory. ACC: MOL.20040303.0023.
- 168471 Gray, W.J. 1988. Effect of Surface Oxidation, Alpha Radiolysis, and Salt Brine Composition on Spent Fuel and UO<sub>2</sub> Leaching Performance. PNL/SRP-6689. Richland, Washington: Pacific Northwest Laboratory. ACC: HQX.19881021.0025.
- Gray, W.J. and Einziger, R.E. 1998. *Initial Results from Dissolution Rate Testing of N-Reactor Spent Fuel Over a Range of Potential Geologic Repository Aqueous Conditions*. DOE/SNF/REP-022, Rev. 0. Washington, D.C.: U.S. Department of Energy. TIC: 245380.
- 149367 Kaplan, I. 1963. *Nuclear Physics*. 2nd edition. Reading, Massachusetts: Addison-Wesley Publishing. TIC: 247872.
- Lam, P.S.; Sindelar, R.L.; and Peacock, H.B. Jr. 1997. *Vapor Corrosion of Aluminum Cladding Alloys and Aluminum-Uranium Fuel Materials in Storage Environments (U)*. WSRC-TR-97-0120. Aiken, South Carolina: Westinghouse Savannah River Company. TIC: 248909.
- 168475 Lawrence, L.A. 1999. K Basin Spent Nuclear Fuel Characterization. HNF-3534, Rev. 0. Richland, Washington: Duke Engineering & Services Hanford, Inc. ACC: MOL.20040325.0053.
- 142133 Lederer, C.M. and Shirley, V.S., eds. 1978. *Table of Isotopes*. 7th Edition. New York, New York: John Wiley & Sons. TIC: 243883.

- 149429 Marschman, S.C.; Pyecha, T.D.; and Abrefah, J. 1997. *Metallographic Examination of Damaged N Reactor Spent Nuclear Fuel Element SFEC5,4378.* PNNL-11438. Richland, Washington: Pacific Northwest National Laboratory. TIC: 248059.
- 158010 McKenzie, D.G., IV. 2002. *Waste Package Design Methodology Report*. TDR-MGR-MD-000006 REV 02. Las Vegas, Nevada: Bechtel SAIC Company. ACC: MOL.20020404.0085.
- NRC (U.S. Nuclear Regulatory Commission) 2003. *Yucca Mountain Review Plan, Final Report*. NUREG-1804, Rev. 2. Washington, D.C.: U.S. Nuclear Regulatory Commission, Office of Nuclear Material Safety and Safeguards. TIC: 254568.
- 103896 Parrington, J.R.; Knox, H.D.; Breneman, S.L.; Baum, E.M.; and Feiner, F. 1996. Nuclides and Isotopes, Chart of the Nuclides. 15th Edition. San Jose, California: General Electric Company and KAPL, Inc. TIC: 233705.
- Propp, W.A. 1998. *Graphite Oxidation Thermodynamics/Reactions*. DOE/SNF/REP-018, Rev. 0. Idaho Falls, Idaho: U.S. Department of Energy. TIC: 247663.
- Quinones, J.; Grambow, B.; Loida, A.; and Geckeis, H. 1996. "Coprecipitation Phenomena During Spent Fuel Dissolution. Part 1: Experimental Procedure and Initial Results on Trivalent Ion Behaviour." *Journal of Nuclear Materials*, 238, ([1]), 38-43. Amsterdam, The Netherlands: Elsevier. TIC: 252663.
- Rechard, R.P., ed. 1995. *Methodology and Results*. Volume 2 of *Performance Assessment of the Direct Disposal in Unsaturated Tuff of Spent Nuclear Fuel and High-Level Waste Owned by U.S. Department of Energy*. SAND94-2563/2. Albuquerque, New Mexico: Sandia National Laboratories. TIC: 237102.
- Reilly, M.A. 1998. *Spent Nuclear Fuel Project Technical Databook*. HNF-SD-SNF-TI-015, Rev. 5. Richland, Washington: Fluor Daniel Hanford. TIC: 247814.
- Sanchez, L.C.; Rath, J.S.; Aguilar, R.; Trellue, H.R.; Cochrane, K.; Taylor, L.L.; and Wilson, J.R. 1998. *Nuclear Dynamics Consequence Analysis (NDCA) for the Disposal of Spent Nuclear Fuel in an Underground Geologic Repository*. DOE/SNF/REP-0033, REV 0. Three Volumes. Washington, D.C.: U.S. Department of Energy. TIC: 247643.
- 159406 Schulz, W.W. 1972. *Shear-Leach Processing of N-Reactor Fuel--Cladding Fires*. ARH-2351. Richland, Washington: Atlantic Richfield Hanford. TIC: 243079.
- Shoesmith, D.W. and Sunder, S. 1992. "The Prediction of Nuclear Fuel (UO<sub>2</sub>) Dissolution Rates Under Waste Disposal Conditions." *Journal of Nuclear Materials*, 190, 20-35. Amsterdam, The Netherlands: Elsevier. TIC: 246431.

- 166960 Simmons, A.M. 2004. *Yucca Mountain Site Description*. TDR-CRW-GS-000001 REV 02. Two volumes. Las Vegas, Nevada: Bechtel SAIC Company. ACC: DOC.20040120.0004.
- Solbrig, C.W.; Krsul, J.R.; and Olsen, D.N. 1994. "Pyrophoricity of Uranium in Long-Term Storage Environments." *Proceedings of the Topical Meeting on DOE Spent Nuclear Fuel—Challenges and Initiatives, Salt Lake City, Utah, December 13-16, 1994.* Pages 89-93. La Grange Park, Illinois: American Nuclear Society. TIC: 103316.
- Sunder, S. and Shoesmith, D.W. 1991. *Chemistry of UO<sub>2</sub> Fuel Dissolution in Relation to the Disposal of Used Nuclear Fuel*. AECL-10395. Pinawa, Manitoba, Canada: Whiteshell Laboratories, Atomic Energy of Canada Limited. TIC: 246920.
- Sunder, S.; Shoesmith, D.W.; and Miller, N.H. 1997. "Oxidation and Dissolution of Nuclear Fuel (UO[sub]2) by the Products of the Alpha Radiolysis of Water." *Journal of Nuclear Materials*, 244, 66-74. Amsterdam, The Netherlands: Elsevier. TIC: 246914.
- Swanson, J.L.; Bray, L.A.; Kjarmo, H.E.; Ryan, J.L.; Matsuzaki, C.L.; Pitman, S.G.; and Haberman, J.H. 1985. *Laboratory Studies of Shear/Leach Processing of Zircaloy Clad Metallic Uranium Reactor Fuel*. PNL--5708. Richland, Washington: Pacific Northwest Laboratory. ACC: MOL.20040325.0049.
- Thornton, T.A. 1998. "HPPP Issue 1; Preliminary TSPA for a Pyrophoric Event Involving N-Reactor SNF Waste Packages." Interoffice correspondence from T.A. Thornton (CRWMS M&O) to J.S. Clouet, S.S. Sareen, and D. Stahl, September 21, 1998, LV.WP.TAT.09/98-179, with attachment. ACC: MOL.19981019.0001.
- Thornton, T.A. 1998. "HPPP Issue 1; Preliminary TSPA for N-Reactor SNF Waste Packages." Interoffice correspondence from T.A. Thornton (CRWMS M&O) to J.S. Clouet, S.S. Sareen, and D. Stahl, June 1, 1998, LV.WP.TAT.05/98-111, with attachment. ACC: MOL.19980730.0142.
- Werme, L.O. and Spahiu, K. 1998. "Direct Disposal of Spent Nuclear Fuel: Comparison Between Experimental and Modelled Actinide Solubiluties in Natural Waters." *Journal of Alloys and Compounds*, 271-273, 194-200. Lausanne, Switzerland: Elsevier. TIC: 243085.
- Wick, O.J., ed. 1980. *Plutonium Handbook: A Guide to the Technology*. Volumes I & II. La Grange Park, Illinois: American Nuclear Society. TIC: 248002.
- Wilson, M.L.; Gauthier, J.H.; Barnard, R.W.; Barr, G.E.; Dockery, H.A.; Dunn, E.; Eaton, R.R.; Guerin, D.C.; Lu, N.; Martinez, M.J.; Nilson, R.; Rautman, C.A.; Robey, T.H.; Ross, B.; Ryder, E.E.; Schenker, A.R.; Shannon, S.A.; Skinner, L.H.; Halsey, W.G.; Gansemer, J.D.; Lewis, L.C.; Lamont, A.D.; Triay, I.R.; Meijer, A.; and Morris, D.E. 1994. *Total-System Performance Assessment for Yucca Mountain SNL Second Iteration (TSPA-1993)*. SAND93-2675. Executive Summary and two

- volumes. Albuquerque, New Mexico: Sandia National Laboratories. ACC: NNA.19940112.0123.
- Wood, D.H.; Snowden, S.A.; Howe, H.J., Jr.; Thomas, L.L.; Moon, D.W.; Gregg, H.R.; and Miller, P.E. 1994. "Regarding the Chemistry of Metallic Uranium Stored in Steel Drums." *Journal of Nuclear Materials*, 209, (1), 113-115. New York, New York: Elsevier. TIC: 255359.
- YMP (Yucca Mountain Site Characterization Project) 2001. *Yucca Mountain Site Characterization Project Requirements Document (YMP-RD)*. YMP/CM-0025, Rev. 4, DCN 02. Las Vegas, Nevada: Yucca Mountain Site Characterization Office. ACC: MOL.20010322.0491; MOL.20011107.0002.

### 8.2 CODES, STANDARDS, REGULATIONS, AND PROCEDURES

- 156605 10 CFR 63. Energy: Disposal of High-Level Radioactive Wastes in a Geologic Repository at Yucca Mountain, Nevada. Readily available.
- 162618 67 FR 19432. Surplus Plutonium Disposition Program. Readily available.
  - AP-2.27Q, Rev. 1, ICN 3. *Planning for Science Activities*. Washington, D.C.: U.S. Department of Energy, Office of Civilian Radioactive Waste Management. ACC: DOC.20040407.0002.
  - AP-3.15Q, Rev. 4, ICN 3. *Managing Technical Product Inputs*. Washington, D.C.: U.S. Department of Energy, Office of Civilian Radioactive Waste Management. ACC: DOC.20040225.0011.
  - AP-SIII.2Q, Rev. 1, ICN 2. *Qualification of Unqualified Data*. Washington, D.C.: U.S. Department of Energy, Office of Civilian Radioactive Waste Management. ACC: DOC.20040127.0008.
  - AP-SIII.9Q, Rev. 1, ICN 4. *Scientific Analyses*. Washington, D.C.: U.S. Department of Energy, Office of Civilian Radioactive Waste Management. ACC: DOC.20040407.0003.
  - AP-SV.1Q, Rev. 1, ICN 1. *Control of the Electronic Management of Information*. Washington, D.C.: U.S. Department of Energy, Office of Civilian Radioactive Waste Management. ACC: DOC.20040308.0001.
- ASTM C 1454-00. 2000. Standard Guide for Pyrophoricity/Combustibility Testing in Support of Pyrophoricity Analyses of Metallic Uranium Spent Nuclear Fuel. West Conshohocken, Pennsylvania: American Society for Testing and Materials. TIC: 248977.
  - LP-SI.11Q-BSC, Rev. 0, ICN 0. *Software Management*. Washington, D.C.: U.S. Department of Energy, Office of Civilian Radioactive Waste Management. ACC: DOC.20040225.0007.

# 8.3 SOURCE DATA, LISTED BY DATA TRACKING NUMBER

- 164527 MO0307SEPFEPS4.000. LA FEP List. Submittal date: 07/31/2003.
- 168762 MO0402SPAHWCIG.002. Heat and Water Chemistry Output from Igneous Intrusion. Submittal date: 02/23/2004.

Miscellaneous Waste-Form FEPs

INTENTIONALLY LEFT BLANK

# 9. ATTACHMENTS

A list of the attachments can be found in Table 9-1.

Table 9-1. List of Attachments

Attachment	Title
I	Analysis of the Potential for Pyrophoric Behavior in DSNF
II	Radionuclide Inventory for Final Waste Forms
III	Alpha Recoil Mechanics
IV	Radionuclide Inventory for Pressurized-Water Reactor Spent Nuclear Fuels and Boiling- Water Reactor Spent Nuclear Fuels
V	Data Qualification For Direct Inputs To Miscellaneous Waste-Form FEPs
VI	Data Qualification Plan (Scanned Images)

Miscellaneous Waste-Form FEPs

INTENTIONALLY LEFT BLANK

#### ATTACHMENT I

## ANALYSIS OF THE POTENTIAL FOR PYROPHORIC BEHAVIOR IN DSNF

The DOE Office of Environmental Management/Office of Civilian Radioactive Waste Management Repository Task Team (DOE 1997 [DIRS 149432], pp. 20-21) has addressed three fuel types with regard to their potential for pyrophoric reactions: oxide, metal, and carbide fuels. A fourth (metallic sodium-bonded fuel) has been eliminated from further consideration because it is a listed RCRA hazard and will be treated prior to repository emplacement. DSNF is only a small part of the total waste inventory in the repository. The characteristics and potential for pyrophoric behavior of these three fuel types are discussed in the following paragraphs.

Oxide fuels consist of U-oxide fuels, Th/U-oxide fuels, and U/Pu-oxide fuels of varying enrichments and concentrations. Bulk UO<sub>2</sub> fuels have been exposed in oxidizing environments at temperatures considerably higher than expected repository temperatures with no indication of ignition. It is not expected that the addition of significant amounts of ThO<sub>2</sub> or PuO<sub>2</sub> in the mixed oxide fuels will make the fuel pyrophoric as long as the matrix form is composed of heavy-metal oxides (DOE 1997 [DIRS 149432], p. 20).

Metallic uranium-based fuels will oxidize in an air or water environment and can be pyrophoric, particularly when in a fine particulate form or when a significant amount of hydride has formed in the uranium metal matrix. The corrosion of uranium metal results in the formation of uranium hydrides as finely dispersed inclusions in the uranium metal. Although examination and testing of damaged N-Reactor zirconium-clad uranium metal fuel showed only small amounts of uranium hydride formed by corrosion as precipitates within the metal and in thin coatings on the internal crack surfaces (Marschman et al. 1997 [DIRS 149429], Section 3.4.2), their presence is believed to be responsible for the observed decreased ignition temperature observed during ignition testing of damaged or corroded N-Reactor SNF samples compared to unirradiated or undamaged samples (Abrefah et al. 1999 [DIRS 151226], Tables 4.2 and 4.3). Additionally, the possibility exists that additional U-hydride will form during interim storage (Reilly 1998 [DIRS 149433], p. 30), which could potentially act as an ignition source if concentrated in a small area.

TRIGA fuel, predominantly composed of U-Zr-hydride, is not as susceptible to pyrophoric reactions as uranium metal fuel because this fuel does not display the extensive damage or corrosion evident in the N-Reactor SNF.

Most aluminum-clad uranium metal DSNF (i.e., fuel located at the Savannah River Site) does not have the amount of damaged/corroded uranium metal (and extent of uranium hydride formation and consequent potential for pyrophoricity) shown by the N-Reactor SNF (Lam et al. 1997 [DIRS 152482], Section 8). The small fraction (e.g., Single-Pass Reactor SNF) of the total aluminum-clad uranium-metal SNF inventory that is currently located in the K-Basins at Hanford could display damage or corrosion characteristics similar to N-Reactor SNF due to its uranium metal core and similar handling and wet-storage history. This aluminum-clad uranium metal SNF will be disposed in the N-Reactor SNF canisters. The TSPA-LA will (conservatively) not differentiate waste packages with MCOs containing this SNF from MCOs containing the N-Reactor SNF.

The U-Mo fuels should behave similarly to the Al-U SNF. The uranium/aluminum alloy matrix fuel is much less reactive than U-metal (DOE 1997 [DIRS 149432], p. 21; DOE 2002 [DIRS 158405], Section 6.2). Because of the low U loading of these U-Mo and most Al-U fuels (less than 9 percent of their total mass is U), it is anticipated that less UH<sub>3</sub> would be present than in the N-Reactor SNF, although this has not been tested experimentally.

Carbide fuels are not a pyrophoric hazard in a dry atmosphere except as high surface area powders. In a moist atmosphere (as would be required to corrode through a waste package), uranium carbide (UC<sub>2</sub>) will react to form UO<sub>2</sub>, carbon dioxide (CO<sub>2</sub>), and hydrocarbon gases. The major constituent of the hydrocarbon gases is methane with minor constituents being ethane, ethylene, and acetylene. These gases are flammable in air, but only acetylene is autocatalytically explosive. An analysis of carbide fuels (Propp 1998 [DIRS 149395]) indicated that the oxidizing environment of the repository would inhibit the formation of hydrocarbons. It should also be noted that less than 1 percent of the DSNF inventory is carbide SNF.

The following conditions were used in this analysis to create a worst case scenario. This worst case scenario will then be used to determine the maximum impact pyrophoricity can have on repository performance. A pyrophoric event cannot occur unless or until:

- The waste package and SNF canister have been breached;
- There is sufficient oxygen available to support a pyrophoric event;
- An ignition source (overheating due to oxidation, spark, mechanical impact, etc.) is available.

The greatest risk of pyrophoric behavior is from the N-Reactor SNF because a significant fraction of the fuel elements have damaged cladding, resulting in the exposure of the damaged and corroded uranium metal cores. Both the N-Reactor and similar types of uranium-metal-based materials have shown pyrophoric behavior in the past (Schulz 1972 [DIRS 159406]; Wood et al. 1994 [DIRS 165884]; Solbrig et al. 1994 [DIRS 165881]). N-Reactor SNF constitutes the large majority of the DSNF (85 percent), but less than approximately 1.3 percent of the total waste to be stored at Yucca Mountain (BSC 2003 [DIRS 163693], Sections 6.4 and 8). A pyrophoric event could result in the nearly instantaneous release of the soluble and volatile radionuclide inventory in the affected packages and the breach of the two adjacent waste packages.

A pyrophoric event can impact a number of repository components: the directly affected waste packages (cladding, fuel, and in-package chemistry), nearby waste packages, and nearby geohydrology. It can be postulated that changes in local percolation rates could result from changes in the surrounding rock strata caused by a pyrophoric event's thermal energy. However, a postclosure pyrophoric event is not possible unless the waste package and the canister holding the N-Reactor SNF (i.e., the multicanister overpack) breach. Therefore, changes in local percolation rates would not impact waste package failure rates. Also, if the postclosure analysis assumes that the complete dissolution of the waste form within a breached waste package occurs within one time step following its breach, changes in local percolation rates would not significantly impact SNF dissolution rates. The use of titanium drip shields will tend to shield

the surrounding geohydrologic system from any sudden release of thermal energy and distribute it along the drift.

The following argument addresses pyrophoricity in terms of both the total radionuclides that could be released due to a pyrophoric event and the effect a pyrophoric event could have on the peak offsite dose. A sensitivity analysis is included to evaluate the effects of clustering.

Impact on Radionuclide Release—During the regulatory period following repository closure, some percentage of the approximately 160 N-Reactor and 12,000 total waste packages (DOE 1998 [DIRS 122980], Table I-1) will fail. For the purpose of estimating the maximum effect on radionuclide release of pyrophoric events in N-Reactor SNF-containing waste packages, it may be conservatively assumed (see Section 5.2.13) that (1) breach of a waste package containing N-Reactor SNF will result in a pyrophoric event that causes the two adjacent waste packages to fail, (2) the various types of waste packages are evenly distributed throughout the repository, and (3) the probability of failure of a waste package containing pyrophoric (i.e., N-Reactor) SNF is the same as that of any other waste package. Therefore, the additional number of waste package failures due to pyrophoric events during the regulatory period can be estimated as follows. If the fraction of failed waste packages is  $F_b$  and the number of waste packages with N-Reactor SNF is  $P_b \times N_{nr}$ . If the probability that a waste package next to a waste package with N-Reactor SNF has failed prior to a pyrophoric event is  $P_b$ , then the number of additional waste packages that fail due to pyrophoric events in the waste packages with N-Reactor SNF can be expressed as:

$$N_{add} = N_{nr} \times F_b \times (1-P_b)$$
 (Eq. I-1)

where  $N_{add}$  is the number of additionally failed packages and the term  $(1-P_b)$  gives the probability that a neighboring package had *not* failed prior to the pyrophoric event. The value of  $P_b$  can be expressed in terms of  $F_b$ . For a fraction of failed packages  $F_b$ , 2 out of  $2/F_b$  packages are failed. For example, if  $F_b = 0.001$ , then 2 out of every 2/(0.001) = 2,000 packages will have failed. The probability that any particular waste package has failed is  $2/(2/F_b) = F_b$ . The probability that a neighboring waste package fails is:

$$P_b = 1/[(2/F_b)-1]$$
 (Eq. I-2)

for each neighbor. Since there are two neighboring packages, the probability that 1 of the 2 packages failed is approximately  $2/[(2/F_b)-1]$ . (The possibility that both neighbors have failed is approximately  $P_b^2$  and is neglected.) The probability that both a waste package and 1 or both of its neighboring packages are failed is:

$$P_b = F_b \times \{2/[(2/F_b)-1]\}$$
 (Eq. I-3)

The probability that a neighboring package has *not* failed prior to failure of the package with N-Reactor SNF is:

$$(1-P_b) = 1-F_b \times \{2/[(2/F_b)-1]\}$$
 (Eq. I-4)

The probability that a failed waste package with N-Reactor SNF neighbors 2 waste packages that have not failed can be used to calculate the number of additional failures possible from

pyrophoric events. The probability that a waste package with N-Reactor SNF has failed is  $(N_{nr}/N_{tot}) \times F_b$ , where  $N_{tot}$  is the total number of waste packages. The probability that the two neighboring packages have not failed is given in Eq. I-4. The fractional increase in failures is:

$$F_{add} = (N_{nr}/N_{tot}) \times F_b \times 2 \times (1-F_b \times \{2/[(2/F_b)-1]\})$$
 (Eq. I-5)

where a factor of 2 is added to account for the induced failure of 2 neighboring waste packages for every failed package with N-Reactor SNF.

Equation I-5 can be used to calculate fractional increases in the number of waste packages failing due to a pyrophoric event for different fractions of failures. There will be approximately 160 waste packages with N-Reactor SNF and 12,000 packages in total. For  $N_{nr}=160$  and  $N_{tot}=12,000.$  For  $F_b=0.001,\,0.01,\,0.1,\,0.2,\,0.5,\,$  and 0.75, Equation I-5 predicts  $F_{add}=0.00003,\,0.00027,\,0.0026,\,0.0051,\,0.0089,\,$  and 0.0020, respectively. The maximum fractional increase predicted by Eq. I-5 is  $F_{add}=0.0089$  for  $F_b=0.48$ . That is, if 48 percent of all waste packages fail, the increase in failed packages due to pyrophoric events is less than 1 percent. Because the various waste package types were considered to be evenly distributed, corresponding increases occur in the total amounts of radionuclides released over the regulatory period due to pyrophoric events for the N-Reactor SNF-containing waste packages (i.e., the maximum increase in radionuclide release is less than 1 percent). Therefore, even under the extremely conservative scenario that all failed waste packages with N-Reactor SNF undergo pyrophoric reaction and cause the two adjacent waste packages to fail, pyrophoricity in N-Reactor SNF-containing waste packages has an insignificant effect on radionuclide release. This supports the exclusion of FEP 2.1.02.08.0A due to low consequence.

**Impact of Pyrophoric Events on Peak Offsite Dose**—The impact a single pyrophoric event would have on peak offsite dose can be bounded by probabilistically assessing the potential worst case release from a failed waste package, in terms of the potential percent increase in radionuclide release. It is independent of any particular repository model.

A pyrophoric event involving a single N-Reactor waste package with the simultaneous failure of the two adjacent CSNF waste packages could result in a peak offsite dose that is equivalent to approximately three times the value of a single waste package failure.

In the event a waste package containing N-Reactor SNF fails and subsequently undergoes a pyrophoric event, the initial release would be approximately three waste package equivalents of radionuclides rather than one waste package equivalent. However, because whether or when a waste package fails is independent of the type of SNF it contains, the probability that any given failed waste package contains N-Reactor SNF is equal to:

$$N_{nr}/N_{tot} = 160/12,000 = 0.013$$
 (Eq. 1-2)

Therefore, the average increase in radionuclide release from the repository due to a pyrophoric event involving a waste package containing N-Reactor SNF can be represented as the probability that the failed waste package contains N-Reactor SNF multiplied by the probability that waste package undergoes a pyrophoric event multiplied by three waste package equivalents (WPE). In the worst case, where every breach of a waste package containing N-Reactor fuel results in a pyrophoric event, the increase is:

(0.013 N-Reactor WP/total WP)(1pyrophoric event per failed N-Reactor WP)(3 WPE) ≈ 0.04 WPE(Eq. I-3)

This represents a 4 percent increase in peak offsite dose above that which would result if pyrophoric events were not possible. This upper bound reflects the assumption that a pyrophoric event will always occur in a breached N-Reactor SNF-containing waste package, and that the adjacent waste packages contain CSNF. Because a pyrophoric event will most likely not occur following an N-Reactor waste package breach, the actual increase is estimated to be much smaller.

Additionally, preliminary postclosure site boundary dose sensitivity analyses have indicated that the increase of the dose rate at the site boundary resulting from the complete release of the radionuclide inventory in waste packages containing N-Reactor SNF during one performance assessment time step is insignificant (Thornton 1998 [DIRS 107796]). Thus, even the postulated instantaneous release due to a pyrophoric event does not have a significant effect on overall radionuclide releases and thus supports the exclusion of FEP 2.1.02.08.0A due to low consequence.

Clustering Sensitivity Model—Clustering can be defined as multiple waste packages failing in a short time period. They can be postulated as being either induced by some initiating event that is not associated with pyrophoricity of DSNF (nonpyrophoric-induced cluster) or induced by an initiating pyrophoric event that results in subsequent pyrophoric events (pyrophoric-induced cluster). Regarding nonpyrophoric-induced clusters, an argument can be made similar to that in the preceding section. Regardless of the number of waste packages involved in some random event that results in clustering of nonpyrophoric event-induced waste package failures, each waste package involved has approximately 0.013 probability of being an N-Reactor waste package. Therefore, the maximum impact pyrophoric events associated with a nonpyrophoric-induced clustering event would be a 4 percent increase in the peak dose reflected in Eq. I-3.

The effect of pyrophoric event-induced clustering event will be insignificant based on the expected separation that will exist between emplaced N-Reactor waste packages. Also, there will likely be insufficient oxygen available in a drift to support multiple pyrophoric events occurring simultaneously.

INTENTIONALLY LEFT BLANK

# ATTACHMENT II RADIONUCLIDE INVENTORY FOR FINAL WASTE FORMS

Sanchez et al. (1998 [DIRS 149368]) estimated the masses of the radionuclides to be disposed of in the Yucca Mountain repository. These values were calculated with use of radioactivity values from *Waste Form Degradation and Radionuclide Mobilization Expert Elicitation Project* (CRWMS M&O 1998 [DIRS 100374]) and are presented below in Table II-1. The significant findings of this table are:

- Of the radionuclide mass to be disposed of in the Yucca Mountain repository, 95.6 percent is anticipated to be due to CSNF. The remaining 4.4 percent of the mass will be comprised of DSNF and HLW.
- The four radionuclides that dominate the total mass inventory are <sup>238</sup>U, <sup>235</sup>U, <sup>239</sup>Pu, and <sup>236</sup>U. Of these, <sup>238</sup>U is the main contributor with 63.9 million kilograms of mass. This corresponds to nearly 97 percent of the total mass from all the radionuclides to be disposed of in the repository.
- When ranking DOE-owned materials by themselves, <sup>232</sup>Th is third behind <sup>238</sup>U and <sup>235</sup>U. This radionuclide, however, is not significant to total inventory. Its presence is due to the existence of Thorium fuel-cycle materials that are unique to DOE-owned fuel.

Table II-1. YMP-Scale Source Term Mass Inventory (Calendar Year = 2035, Time = 0 yr) (a)

	DOE-0	Owned	Comn	nercial	
Nuclide ID	SNF kg (%)	HLW kg (%)	PWR kg (%)	BWR kg (%)	Total (kg)
<sup>227</sup> Ac	4.24E-04 (8.92E+01)	3.91E-05 (8.23E+00)	8.39E-06 (1.76E+00)	3.73E-06 (7.85E-01)	4.76×10 <sup>-4</sup>
<sup>108m</sup> Ag †	0.00E+00 (0.00E+00)	0.00E+00 (0.00E+00)	0.00E+00 (0.00E+00)	0.00E+00 (0.00E+00)	0
<sup>241</sup> Am	3.09E+02 (5.07E-01)	1.19E+02 (1.94E-01)	4.14E+04 (6.79E+01)	1.92E+04 (3.14E+01)	6.1×10 <sup>4</sup>
<sup>242m</sup> Am	8.27E-02 (5.68E-02)	9.25E-03 (6.35E-03)	9.64E+01 (6.62E+01)	4.92E+01 (3.37E+01)	146
<sup>243</sup> Am	9.08E+00 (1.08E-01)	8.68E-01 (1.03E-02)	5.87E+03 (6.96E+01)	2.55E+03 (3.03E+01)	8430
<sup>14</sup> C	2.06E-01 (9.76E-01)	0.00E+00 (0.00E+00)	1.33E+01 (6.32E+01)	7.54E+00 (3.58E+01)	21.1
<sup>36</sup> CI	1.32E-01 (5.86E-01)	0.00E+00 (0.00E+00)	1.50E+01 (6.66E+01)	7.39E+00 (3.28E+01)	22.5
<sup>243</sup> Cm †	0.00E+00 (0.00E+00)	0.00E+00 (0.00E+00)	0.00E+00 (0.00E+00)	0.00E+00 (0.00E+00)	0
<sup>244</sup> Cm	9.54E-01 (6.75E-02)	6.63E-01 (4.69E-02)	1.01E+03 (7.16E+01)	3.99E+02 (2.83E+01)	1410
<sup>245</sup> Cm	1.77E-02 (1.34E-02)	1.54E-03 (1.16E-03)	9.79E+01 (7.38E+01)	3.47E+01 (2.62E+01)	133
<sup>246</sup> Cm	1.68E-02 (1.09E-01)	9.80E-05 (6.38E-04)	1.16E+01 (7.53E+01)	3.78E+00 (2.46E+01)	15.4
<sup>135</sup> Cs	1.77E+02 (5.74E-01)	4.70E+02 (1.52E+00)	2.07E+04 (6.72E+01)	9.46E+03 (3.07E+01)	3.08×10 <sup>4</sup>
<sup>137</sup> Cs	3.94E+02 (7.11E-01)	7.13E+02 (1.29E+00)	3.84E+04 (6.92E+01)	1.60E+04 (2.88E+01)	5.54×10 <sup>4</sup>
<sup>129</sup>	9.28E+01 (7.02E-01)	5.06E-02 (3.83E-04)	9.23E+03 (6.98E+01)	3.90E+03 (2.95E+01)	1.32×10 <sup>4</sup>
<sup>93</sup> Mo †	0.00E+00 (0.00E+00)	0.00E+00 (0.00E+00)	0.00E+00 (0.00E+00)	0.00E+00 (0.00E+00)	0
<sup>93m</sup> Nb ‡	1.17E-07 (5.37E-01)	5.28E-07 (2.43E+00)	1.41E-05 (6.50E+01)	6.96E-06 (3.21E+01)	2.17×10 <sup>-5</sup>
<sup>94</sup> Nb	5.52E-02 (1.87E-02)	7.46E-04 (2.53E-04)	2.84E+02 (9.63E+01)	1.09E+01 (3.71E+00)	295
<sup>59</sup> Ni	6.04E+00 (2.87E-01)	1.67E+00 (7.95E-02)	1.58E+03 (7.51E+01)	5.17E+02 (2.45E+01)	2110

Table II-1. YMP-Scale Source Term Mass Inventory (Calendar Year = 2035, Time = 0 yr) (a) (Continued)

	DOE-0	Dwned	Comn	nercial	
Nuclide ID	SNF kg (%)	HLW kg (%)	PWR kg (%)	BWR kg (%)	Total (kg)
<sup>63</sup> Ni	6.49E+00 (1.75E+00)	0.00E+00 (0.00E+00)	2.79E+02 (7.50E+01)	8.62E+01 (2.32E+01)	371
<sup>237</sup> Np	2.30E+02 (5.55E-01)	1.89E+02 (4.55E-01)	3.01E+04 (7.26E+01)	1.10E+04 (2.64E+01)	4.15×10 <sup>4</sup>
<sup>231</sup> Pa	1.84E+00 (9.29E+01)	9.70E-02 (4.91E+00)	2.94E-02 (1.49E+00)	1.31E-02 (6.65E-01)	1.98
<sup>210</sup> Pb	1.03E-07 (3.15E+01)	1.68E-09 (5.11E-01)	1.53E-07 (4.67E+01)	6.97E-08 (2.12E+01)	3.28×10 <sup>-7</sup>
<sup>107</sup> Pd	5.52E+01 (3.33E-01)	0.00E+00 (0.00E+00)	1.15E+04 (6.96E+01)	4.97E+03 (3.01E+01)	1.65×10 <sup>4</sup>
<sup>238</sup> Pu	3.51E+01 (2.65E-01)	1.10E+02 (8.29E-01)	9.58E+03 (7.23E+01)	3.52E+03 (2.66E+01)	1.33×10 <sup>4</sup>
<sup>239</sup> Pu	6.98E+03 (1.77E+00)	3.59E+02 (9.08E-02)	2.75E+05 (6.96E+01)	1.13E+05 (2.85E+01)	3.95×10 <sup>5</sup>
<sup>240</sup> Pu	1.38E+03 (8.76E-01)	6.80E+01 (4.33E-02)	1.10E+05 (6.98E+01)	4.61E+04 (2.93E+01)	1.57×10 <sup>5</sup>
<sup>241</sup> Pu	6.02E+01 (1.67E-01)	6.76E+00 (1.88E-02)	2.46E+04 (6.83E+01)	1.14E+04 (3.16E+01)	3.60×10 <sup>4</sup>
<sup>242</sup> Pu	6.73E+01 (1.90E-01)	6.18E+00 (1.74E-02)	2.41E+04 (6.81E+01)	1.12E+04 (3.17E+01)	3.54×10 <sup>4</sup>
<sup>226</sup> Ra	7.97E-06 (8.73E+00)	4.46E-07 (4.89E-01)	5.71E-05 (6.25E+01)	2.58E-05 (2.83E+01)	9.13×10 <sup>-5</sup>
<sup>228</sup> Ra ‡	3.63E-05 (1.00E+02)	0.00E+00 (0.00E+00)	3.77E-11 (1.04E-04)	1.58E-11 (4.34E-05)	3.63×10 <sup>-5</sup>
<sup>79</sup> Se	3.40E+00 (7.77E-01)	6.19E+00 (1.42E+00)	3.03E+02 (6.91E+01)	1.25E+02 (2.87E+01)	438
<sup>151</sup> Sm	1.93E+01 (1.93E+00)	0.00E+00 (0.00E+00)	6.88E+02 (6.88E+01)	2.93E+02 (2.93E+01)	1000
<sup>121m</sup> Sn †	0.00E+00 (0.00E+00)	0.00E+00 (0.00E+00)	0.00E+00 (0.00E+00)	0.00E+00 (0.00E+00)	0
<sup>126</sup> Sn	1.11E+01 (5.46E-01)	0.00E+00 (0.00E+00)	1.43E+03 (7.02E+01)	5.95E+02 (2.93E+01)	2030
<sup>90</sup> Sr	2.12E+02 (8.80E-01)	3.13E+02 (1.30E+00)	1.68E+04 (6.95E+01)	6.85E+03 (2.84E+01)	2.41×10 <sup>4</sup>
<sup>99</sup> Tc	4.36E+02 (7.62E-01)	9.13E+02 (1.60E+00)	3.92E+04 (6.86E+01)	1.66E+04 (2.91E+01)	5.72×10 <sup>4</sup>
<sup>229</sup> Th	1.28E-01 (9.97E+01)	3.34E-04 (2.59E-01)	6.96E-05 (5.40E-02)	2.61E-05 (2.03E-02)	0.129
<sup>230</sup> Th	7.23E-02 (8.12E+00)	2.89E-03 (3.24E-01)	5.65E-01 (6.34E+01)	2.51E-01 (2.81E+01)	0.891
<sup>232</sup> Th ‡	7.94E+04 (9.46E+01)	4.51E+03 (5.37E+00)	1.32E-01 (1.58E-04)	5.47E-02 (6.52E-05)	8.39×10 <sup>4</sup>
<sup>232</sup> U †	0.00E+00 (0.00E+00)	0.00E+00 (0.00E+00)	0.00E+00 (0.00E+00)	0.00E+00 (0.00E+00)	0
<sup>233</sup> U	1.24E+03 (9.99E+01)	2.84E-01 (2.29E-02)	2.66E-01 (2.14E-02)	9.57E-02 (7.71E-03)	1240
<sup>234</sup> U	2.67E+02 (1.92E+00)	3.76E+01 (2.70E-01)	9.49E+03 (6.82E+01)	4.13E+03 (2.97E+01)	1.39×10 <sup>4</sup>
<sup>235</sup> U	1.37E+05 (2.06E+01)	1.73E+02 (2.59E-02)	3.64E+05 (5.46E+01)	1.65E+05 (2.48E+01)	6.66×10 <sup>5</sup>
<sup>236</sup> U	1.15E+04 (3.87E+00)	3.17E+01 (1.07E-02)	2.03E+05 (6.82E+01)	8.30E+04 (2.79E+01)	2.97×10 <sup>5</sup>
<sup>238</sup> U	2.60E+06 (4.06E+00)	5.30E+04 (8.29E-02)	4.02E+07 (6.28E+01)	2.11E+07 (3.30E+01)	6.39×10 <sup>7</sup>
<sup>93</sup> Zr	6.24E+02 (9.47E-01)	1.31E+03 (1.99E+00)	4.29E+04 (6.52E+01)	2.10E+04 (3.19E+01)	6.59×10 <sup>4</sup>
Total	2.84E+06 (4.30E+00) <sup>b</sup>	6.23E+04 (9.44E-02) <sup>c</sup>	4.14E+07 (6.28E+01)	2.16E+07 (3.28E+01)	6.60×10 <sup>7</sup>
	2.90E+06 (4.39%)		6.31E+07 (95.6%)		
	Top 10 Radionud	lides (Ranked on Total I	nventory for DOE-Owned	and Commercial)	
<sup>238</sup> U	2.60E+06 (4.06E+00)	5.30E+04 (8.29E-02)	4.02E+07 (6.28E+01)	2.11E+07 (3.30E+01)	6.39×10 <sup>7</sup>
<sup>235</sup> U	1.37E+05 (2.06E+01)	1.73E+02 (2.59E-02)	3.64E+05 (5.46E+01)	1.65E+05 (2.48E+01)	6.66×10 <sup>5</sup>
<sup>239</sup> Pu	6.98E+03 (1.77E+00)	3.59E+02 (9.08E-02)	2.75E+05 (6.96E+01)	1.13E+05 (2.85E+01)	3.95×10 <sup>5</sup>
<sup>236</sup> U	1.15E+04 (3.87E+00)	3.17E+01 (1.07E-02)	2.03E+05 (6.82E+01)	8.30E+04 (2.79E+01)	2.97×10 <sup>5</sup>
<sup>240</sup> Pu	1.38E+03 (8.76E-01)	6.80E+01 (4.33E-02)	1.10E+05 (6.98E+01)	4.61E+04 (2.93E+01)	1.57×10 <sup>5</sup>
<sup>232</sup> Th ‡	7.94E+04 (9.46E+01)	4.51E+03 (5.37E+00)	1.32E-01 (1.58E-04)	5.47E-02 (6.52E-05)	8.39×10 <sup>4</sup>
<sup>93</sup> Zr	6.24E+02 (9.47E-01)	1.31E+03 (1.99E+00)	4.29E+04 (6.52E+01)	2.10E+04 (3.19E+01)	6.59×10 <sup>4</sup>
<sup>241</sup> Am	3.09E+02 (5.07E-01)	1.19E+02 (1.94E-01)	4.14E+04 (6.79E+01)	1.92E+04 (3.14E+01)	6.10×10 <sup>4</sup>
<sup>99</sup> Tc	4.36E+02 (7.62E-01)	9.13E+02 (1.60E+00)	3.92E+04 (6.86E+01)	1.66E+04 (2.91E+01)	5.72×10 <sup>4</sup>

YMP-Scale Source Term Mass Inventory (Calendar Year = 2035, Time = 0 yr) (a) (Continued) Table II-1.

	DOE-0	Owned	Comn	nercial	
Nuclide ID	SNF kg (%)	HLW kg (%)	PWR kg (%)	BWR kg (%)	Total (kg)
<sup>137</sup> Cs	3.94E+02 (7.11E-01)	7.13E+02 (1.29E+00)	3.84E+04 (6.92E+01)	1.60E+04 (2.88E+01)	5.54×10 <sup>4</sup>
	Top 10 Radi	onuclides (Ranked on In	ventory for DOE-Owned	Wastes Only)	
<sup>238</sup> U	2.60E+06 (4.06E+00)	5.30E+04 (8.29E-02)			2.65×10 <sup>6</sup>
<sup>235</sup> U	1.37E+05 (2.06E+01)	1.73E+02 (2.59E-02)			1.37×10 <sup>5</sup>
<sup>232</sup> Th ‡	7.94E+04 (9.46E+01)	4.51E+03 (5.37E+00)			8.39×10 <sup>4</sup>
<sup>236</sup> U	1.15E+04 (3.87E+00)	3.17E+01 (1.07E-02)			1.15×10 <sup>4</sup>
<sup>239</sup> Pu	6.98E+03 (1.77E+00)	3.59E+02 (9.08E-02)			7340
<sup>93</sup> Zr	6.24E+02 (9.47E-01)	1.31E+03 (1.99E+00)			1930
<sup>240</sup> Pu	1.38E+03 (8.76E-01)	6.80E+01 (4.33E-02)	<u>——</u>		1450
<sup>99</sup> Tc	4.36E+02 (7.62E-01)	9.13E+02 (1.60E+00)			1350
<sup>233</sup> U	1.24E+03 (9.99E+01)	2.84E-01 (2.29E-02)			1240
<sup>137</sup> Cs	3.94E+02 (7.11E-01)	7.13E+02 (1.29E+00)			1110
	Top 10 Rad	ionuclides (Ranked on I	nventory for Commercia	SNFS Only)	
<sup>238</sup> U			4.02E+07 (6.28E+01)	2.11E+07 (3.30E+01)	6.13×10 <sup>7</sup>
<sup>235</sup> U			3.64E+05 (5.46E+01)	1.65E+05 (2.48E+01)	5.29×10 <sup>5</sup>
<sup>239</sup> Pu			2.75E+05 (6.96E+01)	1.13E+05 (2.85E+01)	3.88×10 <sup>5</sup>
<sup>236</sup> U			2.03E+05 (6.82E+01)	8.30E+04 (2.79E+01)	2.86×10 <sup>5</sup>
<sup>240</sup> Pu			1.10E+05 (6.98E+01)	4.61E+04 (2.93E+01)	1.56×10 <sup>5</sup>
<sup>93</sup> Zr			4.29E+04 (6.52E+01)	2.10E+04 (3.19E+01)	6.39×10 <sup>4</sup>
<sup>241</sup> Am			4.14E+04 (6.79E+01)	1.92E+04 (3.14E+01)	6.06×10 <sup>4</sup>
<sup>99</sup> Tc			3.92E+04 (6.86E+01)	1.66E+04 (2.91E+01)	5.58×10 <sup>4</sup>
<sup>137</sup> Cs			3.84E+04 (6.92E+01)	1.60E+04 (2.88E+01)	5.44×10 <sup>4</sup>
<sup>241</sup> Pu			2.46E+04 (6.83E+01)	1.14E+04 (3.16E+01)	3.60×10 <sup>4</sup>

NOTES: † Data Values for radionuclides were previously reported in Wilson et al. (1994 [DIRS 100191]).

<sup>‡</sup> Data Values for radionuclides were not previously reported in Wilson et al. (1994 [DIRS 100191]).

Table after Sanchez et al. (1998 [DIRS 149368]), data for spent nuclear fuel (SNF) and high-level radioactive waste (HLW) inventory data originally taken from INEEL/PA Parameters Database (DOE 1998 [DIRS 122980]) (values represent intermediate database values, upgraded values can be found in Attachment II). (In total 41 radionuclides are inventoried in DOE (1998 [DIRS 122980]).

b Mass inventory values calculated using half-lives from the Decay Libraries from ORIGEN2 (Croff 1980 [DIRS 142613]; Croff 1980 [DIRS 101554]).

Note, the total DOE-owned mass load (due to radionuclides) is only 2.90E+06 kg. Thus only 4.39% of the total mass load (due to radionuclides) in YMP is due to DOE-Owned inventory.

d Note, the total commercial mass load (due to radionuclides) is 6.30E+07 kg. Thus 95.6% of the total mass load (due to radionuclides) in YMP is due to commercial inventory.

INTENTIONALLY LEFT BLANK

# ATTACHMENT III ALPHA RECOIL MECHANICS

The alpha recoil is analyzed per conservation of momentum in the center-of-mass (COM) frame of reference. Consider Figure III-1; a radionuclide X (e.g.,  $^{238}U$ ), at rest in the lab-system frame of reference (and also in the COM frame), undergoes an alpha decay. The radionuclide X decays to radionuclide Y (e.g.,  $^{234}Th$ ) by emitting an alpha particle, (see Figure III-2 for COM frame).

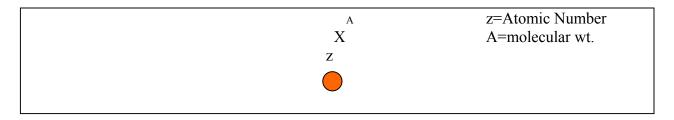


Figure III-1. Initial Center-of-Mass (COM) Frame Conditions for Alpha Emitting Radionuclide

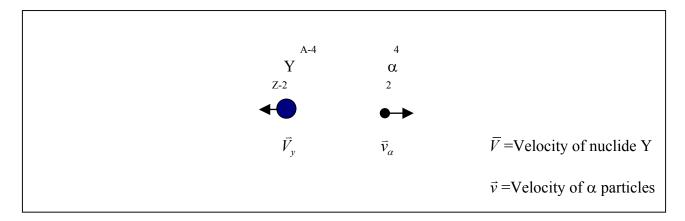


Figure III-2. Final Center-of-Mass (COM) Frame Conditions after Alpha Decay Resulting in Two Decay Products, an Alpha Particle and the Decay Daughter

Applying the conservation of momentum in the COM system leads to Equations III-1 and III-2.

$$0 = M_{\nu} \vec{V}_{\nu} + m_{\alpha} \vec{v}_{\alpha}$$
 (Eq. III-2)

where

 $M_y$  = Mass of recoil nucleus  $m_\alpha$  = Mass of  $\alpha$  particles

Therefore, the velocity of the recoil nucleus (in terms of the velocity of the alpha particle) is:

$$V_y = -v_\alpha \left(\frac{m_\alpha}{M_y}\right)$$
 (Eq. III-3)

where

 $m_{\alpha}$  = mass of the alpha particle  $M_{y}$  = mass of the recoil nucleus.

The kinetic energy of the recoil nucleus can now be determined in terms of the kinetic energy of the emitted alpha particle as:

$$KE(Y) = \frac{1}{2} M_Y V_Y^2 = \frac{m_\alpha}{M_Y} \left( \frac{1}{2} m_\alpha V_\alpha^2 \right) = \frac{m_\alpha}{M_Y} KE(\alpha)$$
(Eq. III-4)

Thus, the kinetic energy of the recoil nucleus is a small fraction of that given to the alpha particle. The energy of the alpha particle is dependent upon the proper mass defect value (the amount of mass converted into energy). For the case of  $^{238}$ U decaying to  $^{234}$ Th, there is:  $KE(\alpha) = 4.196$  MeV (Lederer and Shirley 1978 [DIRS 142133]),  $m_{\alpha} \approx 4.0$ ,  $M_{Th} \approx 234.0$ . This results in a kinetic energy value of 0.072 MeV for the recoil nucleus.

It is important to note that 1) the velocity of the recoil nucleus is in the opposite direction of the alpha particle, and 2) the velocities of both the alpha particle and recoil nucleus are not a function of direction (i.e. they are isotropic in direction in the COM frame). Because the COM is not moving with respect to the lab-system frame, the velocities are also isotropic in the lab-system frame. Thus, for any recoil nucleus moving in a given direction (towards the subsurface groundwater, etc.), there is an equal probability that another recoil nucleus is moving in the opposite direction with the same speed. This isotropy means that only one half of the recoil nuclei are initially moving away from the fuel and into the groundwater.

#### ATTACHMENT IV

# RADIONUCLIDE INVENTORY FOR PRESSURIZED-WATER REACTOR SPENT NUCLEAR FUELS AND BOILING-WATER REACTOR SPENT NUCLEAR FUELS

This attachment contains time-dependent radionuclide information for CSNF with average burnup histories. *Project Requirements Document* (Canori and Leitner 2003 [DIRS 166275], p. 2-53) states that the Yucca Mountain Project shall comply with the relevant requirements contained in *Yucca Mountain Site Characterization Project Requirements Document (YMP-RD)* (YMP 2001 [DIRS 156713]). Table 1.3-1 of YMP-RD (YMP 2001 [DIRS 156713], p. 1.3-6) lists the amount of SNL/HLW to be accepted in the first MGR: 63,000 MTHM CSNF, 640 MTHM commercial HLW, 4,027 MTHM DHLW, and 2,333 MTHM DSNF.

CSNF has considerably higher burnup than that expected for DSNF (e.g., DOE N-Reactor fuels typically have less than one-twentieth of the burnup of CSNF). Table IV-1 presents radionuclide inventories for pressurized-water reactors (PWRs) at various decay times (time after burnup). Table IV-2 presents radionuclide inventories for boiling-water reactors (BWRs) at the same decay times used in Table IV-1. The data for both tables was obtained from PWR Source Term Generation and Evaluation (CRWMS M&O 1999 [DIRS 136429]) and BWR Source Term Generation and Evaluation (CRWMS M&O 1999 [DIRS 136428]). In each table only a limited portion of the original data (timeframes from 125 years up to 10,025 years) is reproduced. The only additions to the tables are: 1) presentation of decay mode and half-lives for the radionuclides in columns 2 and 3, and 2) the generation of the total radionuclide inventories at the bottom of each table. The decay modes and the half-lives were obtained from Parrington et al. (1996 [DIRS 103896]), which demonstrates qualitatively that a significant portion of the radionuclides in the expected inventory are alpha emitters. For simplicity, the net results presented in Table IV-3 present bounding calculations. That is, the calculations consider 100 percent of the radionuclides to be alpha emitters, which are the worst case radiolysis generators. The only numerical values from these tables that are used in Table IV-3 are those for the total radionuclide inventory for the PWR and BWR fuel assemblies (see bottom on Tables IV-1 and IV-2). As can be identified when comparing the final results in Table IV-3 (corrosion rates due to alpha radiolysis) to the dissolution rates in Figure 2, the radiolysis rates are insignificant. This means that if future estimates for the quantities of radionuclides in Tables IV-1 and IV-2 result in slightly different inventories, their differences will not significantly impact the screening argument for FEP 2.1.13.02.0A, Radiation damage in EBS.

Table IV-1. Yucca Mountain Project Radionuclide Inventory for Pressurized-Water Reactor Fuels

Nuclide	Decay	(q) -3: 1 31-11				Radioactivity	Radioactivity Inventory [Ci/Assembly]	Ci/Assembly]			
ID	Mode <sup>(a)</sup>	нап-спе	125 yr	225 yr	325 yr	425 yr	525 yr	1,025 yr	2,025 yr	5,025 yr	10,025 yr
<sup>227</sup> Ac	$\alpha, \beta^-, \gamma$	21.77 years	4.00E-05	5.59E-05	7.14E-05	8.70E-05	1.03E-04	1.85E-04	3.41E-04	8.09E-04	1.59E-03
108Ag	$\beta$ -, $\gamma$ , $\epsilon\beta$ <sup>+</sup>	2.39 minutes	2.23E-04	1.29E-04	7.48E-05	4.34E-05	2.51E-05	1.64E-06	6.99E-09	5.41E-16	7.61E-28
108mAg	$\gamma$ , $\epsilon \beta^+$ , $ITe^-$	130 years	2.56E-03	1.48E-03	8.60E-04	4.98E-04	2.89E-04	1.88E-05	8.03E-08	6.22E-15	8.74E-27
<sup>241</sup> Am	$\alpha, \gamma, \Sigma \Phi$	432.7 years	2.40E+03	2.05E+03	1.75E+03	1.49E+03	1.27E+03	5.69E+02	1.15E+02	1.15E+00	1.36E-01
<sup>242</sup> Am	$\beta^-$ , $\gamma$ , $\epsilon e^-$	16.02 hours	3.89E+00	2.38E+00	1.45E+00	8.90E-01	5.44E-01	4.66E-02	3.42E-04	1.34E-10	2.84E-21
<sup>242m</sup> Am	$\alpha, \gamma, ITe^-, SF$	141 years	3.91E+00	2.39E+00	1.46E+00	8.94E-01	5.47E-01	4.68E-02	3.43E-04	1.35E-10	2.86E-21
<sup>243</sup> Am	$\alpha, \gamma, SF$	7370 years	2.18E+01	2.16E+01	2.14E+01	2.12E+01	2.10E+01	2.00E+01	1.82E+01	1.37E+01	8.57E+00
39Ar	β_	269 years	4.04E-05	3.12E-05	2.41E-05	1.86E-05	1.44E-05	3.97E-06	3.02E-07	1.32E-10	3.36E-16
137mBa	IT	2.552 minutes	3.85E+03	3.82E+02	3.79E+01	3.76E+00	3.73E-01	3.58E-06	3.30E-16	0.00E+00	0.00E+00
<sup>211</sup> Bi	$\alpha, \beta^-, \gamma$	2.14 minutes	4.00E-05	5.59E-05	7.14E-05	8.70E-05	1.03E-04	1.85E-04	3.41E-04	8.09E-04	1.59E-03
<sup>212</sup> Bi	$\alpha, \beta^-, \gamma$	1.009 hours	7.81E-03	2.89E-03	1.07E-03	3.98E-04	1.48E-04	1.91E-06	8.94E-07	9.08E-07	9.37E-07
14C	β_	5730 years	3.28E-01	3.24E-01	3.21E-01	3.17E-01	3.13E-01	2.95E-01	2.61E-01	1.82E-01	9.91E-02
<sup>41</sup> Ca	3	1.03×10 <sup>5</sup> years	9.24E-05	9.24E-05	9.23E-05	9.22E-05	9.22E-05	9.19E-05	9.12E-05	8.94E-05	8.65E-05
113mCd	$\beta^-$ , IT	14.1 years	5.61E-02	4.12E-04	3.02E-06	2.21E-08	1.62E-10	3.43E-21	0.00E+00	0.00E+00	0.00E+00
<sup>142</sup> Ce	β <sup>-</sup> , γ	Stable	1.86E-05	1.86E-05	1.86E-05	1.86E-05	1.86E-05	1.86E-05	1.86E-05	1.86E-05	1.86E-05
<sup>144</sup> Ce	$\alpha, \gamma, SF$	284.6 days	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
<sup>249</sup> Cf	$\alpha, \gamma, SF$	351 years	6.34E-05	5.20E-05	4.27E-05	3.50E-05	2.87E-05	1.07E-05	1.48E-06	3.92E-09	1.99E-13
<sup>250</sup> Cf	$\beta^-,  \beta^+,  \epsilon$	13.1 years	4.20E-07	2.10E-09	1.06E-11	1.55E-13	1.03E-13	1.01E-13	9.67E-14	8.58E-14	7.03E-14
<sub>3e</sub> Cl	$\alpha, \gamma, SF$	3.01×10 <sup>5</sup> years	6.80E-03	6.80E-03	6.80E-03	6.79E-03	6.79E-03	6.79E-03	6.77E-03	6.72E-03	6.65E-03
<sup>242</sup> Cm	$\alpha, \gamma, SF, \varepsilon$	1.2×10 <sup>3</sup> years	3.22E+00	1.97E+00	1.20E+00	7.36E-01	4.50E-01	3.85E-02	2.82E-04	1.12E-10	2.36E-21
<sup>243</sup> Cm	$\alpha, \gamma, SF$	162.8 days	9.01E-01	7.91E-02	6.95E-03	6.10E-04	5.36E-05	2.80E-10	7.66E-21	0.00E+00	0.00E+00
<sup>244</sup> Cm	$\alpha, \gamma, SF$	29.1 years	2.96E+01	6.42E-01	1.40E-02	3.03E-04	6.58E-06	3.18E-14	7.30E-31	0.00E+00	0.00E+00
<sup>245</sup> Cm	$\alpha, \gamma, SF$	18.1 years	3.04E-01	3.02E-01	2.99E-01	2.97E-01	2.94E-01	2.83E-01	2.60E-01	2.04E-01	1.36E-01
<sup>246</sup> Cm	$\beta^-$ , $\gamma$	8.5×10 <sup>3</sup> years	1.03E-01	1.01E-01	9.98E-02	9.83E-02	9.69E-02	9.01E-02	7.78E-02	5.01E-02	2.41E-02
°O <sub>09</sub>	β <sup>-</sup> , γ, ε	4.76×10 <sup>3</sup> years	6.06E-04	1.17E-09	2.27E-15	4.40E-21	8.52E-27	0.00E+00	0.00E+00	0.00E+00	0.00E+00
<sup>134</sup> Cs	β_	5.271 years	6.33E-14	1.59E-28	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
135Cs	β <sup>-</sup> , γ	2.065 years	3.50E-01	3.50E-01	3.50E-01	3.50E-01	3.50E-01	3.50E-01	3.50E-01	3.49E-01	3.49E-01
<sup>137</sup> Cs	γ, ε	2.3×10 <sup>6</sup> years	4.08E+03	4.05E+02	4.01E+01	3.98E+00	3.95E-01	3.79E-06	3.49E-16	0.00E+00	0.00E+00

IV-2 of IV-10

ANL-WIS-MD-000009 REV 01

Table IV-1. Yucca Mountain Project Radionuclide Inventory for Pressurized-Water Reactor Fuels (Continued)

2	Decay	(q) '3: 1 31 ° 1 1				Radioactivit	y Inventory [t	Radioactivity Inventory [Ci/Assembly]			
)	$Mode^{(a)}$	нап-сте	125 yr	225 yr	325 yr	425 yr	525 yr	1,025 yr	2,025 yr	5,025 yr	10,025 yr
<sup>150</sup> Eu	$\beta^-, \gamma, \epsilon \beta^+$	36 years	2.99E-06	4.31E-07	6.23E-08	8.98E-09	1.30E-09	8.11E-14	3.17E-22	0.00E+00	0.00E+00
<sup>152</sup> Eu	$\beta^-$ , $\gamma$ , $\epsilon\gamma$	13.48 years	7.23E-03	3.98E-05	2.20E-07	1.21E-09	6.67E-12	3.39E-23	0.00E+00	0.00E+00	0.00E+00
<sup>154</sup> Eu	$\beta^-$ , $\gamma$	8.59 years	2.10E-01	6.57E-05	2.06E-08	6.44E-12	2.01E-15	0.00E+00	0.00E+00	0.00E+00	0.00E+00
<sup>155</sup> Eu	3	4.71 years	1.90E-05	7.04E-12	2.60E-18	9.61E-25	3.65E-31	0.00E+00	0.00E+00	0.00E+00	0.00E+00
<sub>55</sub> Fe	$\beta^-$	2.73 years	3.25E-11	3.04E-22	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
$H_{\!\scriptscriptstyle \mathrm{E}}$	$\beta^-$ , $\gamma$	12.3 years	4.10E-01	1.48E-03	5.37E-06	1.94E-08	7.02E-11	4.35E-23	0.00E+00	0.00E+00	0.00E+00
<sub>166т</sub> Но	$\beta^-$ , $\gamma$	1.2×10 <sup>3</sup> years	5.08E-04	4.79E-04	4.52E-04	4.27E-04	4.03E-04	3.02E-04	1.69E-04	2.99E-05	1.67E-06
129 <sub>1</sub>	$\beta^-$ , $\gamma$	1.57×10 <sup>7</sup> years	2.19E-02	2.19E-02	2.19E-02	2.19E-02	2.19E-02	2.19E-02	2.19E-02	2.19E-02	2.19E-02
85Kr	γ, ε, ε	10.73 years	1.76E+00	2.74E-03	4.26E-06	6.63E-09	1.03E-11	9.36E-26	0.00E+00	0.00E+00	0.00E+00
<sub>93</sub> Mo	$\beta^+$ , $\epsilon$	~3.5×10³ years	4.06E-02	3.98E-02	3.90E-02	3.83E-02	3.75E-02	3.40E-02	2.79E-02	1.54E-02	5.71E-03
<sub>91</sub> Nb	$ITe^-$	7×10² years	1.77E-05	1.60E-05	1.44E-05	1.30E-05	1.18E-05	7.06E-06	2.55E-06	1.20E-07	7.32E-10
qN <sub>mE6</sub>	$\beta^-$ , $\gamma$	16.1 years	1.09E+00	9.29E-01	9.27E-01	9.26E-01	9.25E-01	9.22E-01	9.16E-01	9.05E-01	8.95E-01
94Nb	3	2.0×10 <sup>4</sup> years	8.36E-01	8.33E-01	8.30E-01	8.28E-01	8.25E-01	8.11E-01	7.84E-01	7.07E-01	5.96E-01
iN <sub>69</sub>	β-	7.6×10 <sup>4</sup> years	2.09E+00	2.09E+00	2.08E+00	2.08E+00	2.08E+00	2.07E+00	2.05E+00	2.00E+00	1.90E+00
<sub>63</sub> Ni	$\alpha, \gamma$	100 years	1.26E+02	6.30E+01	3.15E+01	1.58E+01	7.89E+00	2.47E-01	2.43E-04	2.31E-13	2.12E-28
<sup>237</sup> Np	$\beta^-$ , $\gamma$	2.14×10 <sup>6</sup> years	3.26E-01	3.98E-01	4.60E-01	5.12E-01	5.57E-01	6.98E-01	7.90E-01	8.12E-01	8.11E-01
<sub>238</sub> Np	$\alpha, \beta^-, \gamma$	2.117 days	1.76E-02	1.08E-02	6.58E-03	4.02E-03	2.46E-03	2.11E-04	1.54E-06	6.08E-13	1.29E-23
<sub>239</sub> Np	$\beta^-, \gamma$	1.2×10 <sup>3</sup> years	2.18E+01	2.16E+01	2.14E+01	2.12E+01	2.10E+01	2.00E+01	1.82E+01	1.37E+01	8.57E+00
<sup>231</sup> Pa	$\alpha, \gamma$	3.28×10 <sup>4</sup> years	4.53E-05	6.08E-05	7.63E-05	9.18E-05	1.07E-04	1.85E-04	3.41E-04	8.09E-04	1.59E-03
<sup>233</sup> Pa	$\beta^-$ , $\gamma$	27.0 days	3.26E-01	3.98E-01	4.60E-01	5.12E-01	5.57E-01	6.98E-01	7.90E-01	8.12E-01	8.11E-01
<sup>234</sup> Pa	$\beta^-, \gamma$	6.69 hours	1.92E-04	1.92E-04	1.92E-04	1.92E-04	1.92E-04	1.92E-04	1.92E-04	1.92E-04	1.92E-04
<sup>234m</sup> Pa	$\beta^-, \gamma, IT$	1.17 minutes	1.48E-01	1.48E-01	1.48E-01	1.48E-01	1.48E-01	1.48E-01	1.48E-01	1.48E-01	1.48E-01
<sup>211</sup> Pb	$\beta^-, \gamma$	36.1 minutes	4.00E-05	5.59E-05	7.14E-05	8.70E-05	1.03E-04	1.85E-04	3.41E-04	8.09E-04	1.59E-03
<sup>212</sup> Pb	$\beta^-, \gamma$	10.64 hours	7.81E-03	2.89E-03	1.07E-03	3.98E-04	1.48E-04	1.91E-06	8.94E-07	9.08E-07	9.37E-07
<sup>107</sup> Pd	β-	6.5×10 <sup>6</sup> years	8.41E-02	8.41E-02	8.41E-02	8.41E-02	8.41E-02	8.41E-02	8.41E-02	8.41E-02	8.40E-02
<sup>145</sup> Pm	α, γ, ε	17.7 years	2.13E-05	4.24E-07	8.45E-09	1.68E-10	3.35E-12	1.05E-20	0.00E+00	0.00E+00	0.00E+00
<sup>146</sup> Pm	β-, γ, εγ	5.53 years	4.22E-07	1.52E-12	5.45E-18	1.96E-23	7.03E-29	0.00E+00	0.00E+00	0.00E+00	0.00E+00

IV-3 of IV-10

ANL-WIS-MD-000009 REV 01

Table IV-1. Yucca Mountain Project Radionuclide Inventory for Pressurized-Water Reactor Fuels (Continued)

Mode θ (a, y, y)         Half-Life (a, y, y)         128 yr         228 yr         425 yr         425 yr         1025 yr         2025 yr         1025 yr         2025 yr         1025 yr         2028 yr         2025	Nuclide	Decay	(q) -3: 1 31 - 1 1				Radioactivit	Radioactivity Inventory [Ci/Assembly]	Si/Assembly]			
β. γ         2 6234 years         3.98E-10         1.33E-21         0.00E+00	Q	Mode <sup>(a)</sup>	нап-спе	125 yr	225 yr	325 yr	425 yr	525 yr	1,025 yr	2,025 yr	5,025 yr	10,025 yr
α, β, γ, γ         1 (228 ms)         5 (00E-03)         1 (85E-04)         2 (55E-04)         9 (47E-05)         1 (12E-06)         5 (13E-04)         3 (13E	<sup>147</sup> Pm	β <sup>-</sup> , γ	2.6234 years	3.99E-10	1.33E-21	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
α, β, γ         1.780 ms         4.00e-05         5.59e-05         7.14e-05         1.03e-04         1.85e-04         3.41e-04	<sup>212</sup> Po	α	0.298 ms	5.00E-03	1.85E-03	6.87E-04	2.55E-04	9.47E-05	1.22E-06	5.73E-07	5.81E-07	6.00E-07
α, γ         0.145 seconds         7.81E-03         1.07E-03         3.98E-04         1.48E-04         1.91E-06         0.00E+00           β, γ         17.28 minutes         0.00E+00         0.00E+00 <td< th=""><th><sup>215</sup>Po</th><th><math>\alpha, \beta^-, \gamma</math></th><th>1.780 ms</th><th>4.00E-05</th><th>5.59E-05</th><th>7.14E-05</th><th>8.70E-05</th><th>1.03E-04</th><th>1.85E-04</th><th>3.41E-04</th><th>8.09E-04</th><th>1.59E-03</th></td<>	<sup>215</sup> Po	$\alpha, \beta^-, \gamma$	1.780 ms	4.00E-05	5.59E-05	7.14E-05	8.70E-05	1.03E-04	1.85E-04	3.41E-04	8.09E-04	1.59E-03
$\beta$ , $\gamma$ 17.28 minutes         0.00E+00	<sup>216</sup> Po	α, γ	0.145 seconds	7.81E-03	2.89E-03	1.07E-03	3.98E-04	1.48E-04	1.91E-06	8.94E-07	9.08E-07	9.37E-07
α, γ, SF         2,87 years         8.86E-07         8.85E-07         8.84E-07         8.84E-07         8.81E-07         8.70E-07           α, γ, SF         87.7 years         1.04E+03         4.73E+02         2.16E+02         9.83E+01         4.49E+01         9.43E-01         6.33E-04           α, γ, SF         2.410x10⁴         1.77E+02         1.76E+02         1.76E+02         1.75E+02         1.73E+02         1.69E-07           α, γ, SF         6.56×10³         3.18E+02         3.12E+02         3.09E+02         2.90E+02         2.90E+02         1.69E+02           α, γ         14.4 years         1.64E+00	<sup>144</sup> Pr	β <sup>-</sup> , γ	17.28 minutes	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
$\alpha, \gamma, SF$ $87.7$ years $1.04E+03$ $4.73E+02$ $2.16E+02$ $9.83E+01$ $4.49E+01$ $9.43E-01$ $6.33E-04$ $\alpha, \gamma, SF$ $2.410 \times 10^4$ $1.77E+02$ $1.77E+02$ $1.70E+02$	<sup>236</sup> Pu	$\alpha, \gamma, SF$	2.87 years	8.86E-07	8.85E-07	8.85E-07	8.84E-07	8.84E-07	8.81E-07	8.76E-07	8.60E-07	8.35E-07
$\alpha, \gamma, SF$ $2.410 \times 10^4$ $1.77E+02$ $1.77E+02$ $1.76E+02$ $1.75E+02$ $1.77E+02$ $1$	<sup>238</sup> Pu	$\alpha, \gamma, SF$	87.7 years	1.04E+03	4.73E+02	2.16E+02	9.83E+01	4.49E+01	9.43E-01	6.33E-04	2.97E-10	6.27E-21
$\alpha, \gamma, SF$ $6.66 \times 10^3$ $3.18E + 02$ $3.15E + 02$ $3.12E + 02$ $3.05E + 02$ $3.05E + 02$ $2.05E + 02$ $2.05E + 02$ $2.0E + 02$ </th <th><sup>239</sup>Pu</th> <th><math>\alpha, \gamma, SF</math></th> <th>2.410×10<sup>4</sup></th> <th>1.77E+02</th> <th>1.77E+02</th> <th>1.76E+02</th> <th>1.76E+02</th> <th>1.75E+02</th> <th>1.73E+02</th> <th>1.69E+02</th> <th>1.56E+02</th> <th>1.37E+02</th>	<sup>239</sup> Pu	$\alpha, \gamma, SF$	2.410×10 <sup>4</sup>	1.77E+02	1.77E+02	1.76E+02	1.76E+02	1.75E+02	1.73E+02	1.69E+02	1.56E+02	1.37E+02
α, β·γ         144 years         1.97E+02         1.87E+00         3.12E-01         2.95E-01         2.95E-01         2.85E-01         2.61E-01           α, γ, SF         3.75×10 <sup>5</sup> years         1.64E+00         1.66E+00         1.66E+00         1.66E+00         1.66E+00         1.66E+00	<sup>240</sup> Pu	$\alpha, \gamma, SF$	$6.56 \times 10^3$	3.18E+02	3.15E+02	3.12E+02	3.09E+02	3.05E+02	2.90E+02	2.61E+02	1.90E+02	1.12E+02
$\alpha_{1}\gamma_{1}$ SF         3.75×10 <sup>3</sup> years         1.64E+00         1.64E	<sup>241</sup> Pu	$\alpha, \beta^-, \gamma$	14.4 years	1.97E+02	1.87E+00	3.12E-01	2.97E-01	2.95E-01	2.83E-01	2.61E-01	2.04E-01	1.36E-01
$\alpha_{,\gamma}$ 11.435 days         4.00E-05         5.59E-05         7.14E-05         8.70E-05         1.03E-04         1.85E-04         3.41E-04         3.41E-04 $\alpha_{,\gamma}$ 3.66 days         7.81E-03         2.89E-03         1.07E-03         3.98E-04         1.48E-04         1.91E-06         8.94E-07 $\beta_{,\gamma}$ 4.88×10 <sup>10</sup> years         1.39E-05	<sup>242</sup> Pu	$\alpha, \gamma, SF$	3.75×10 <sup>5</sup> years	1.64E+00	1.64E+00	1.64E+00	1.64E+00	1.64E+00	1.64E+00	1.63E+00	1.62E+00	1.61E+00
α, γ         3.66 days         7.81E-03         2.89E-03         1.07E-03         3.98E-04         1.48E-04         1.91E-06         8.94E-07           β <sup>-</sup> 4.88×10 <sup>10</sup> years         1.39E-05         1.39E-05 <td< th=""><th><sup>223</sup>Ra</th><th><math>\alpha, \gamma</math></th><th>11.435 days</th><th>4.00E-05</th><th>5.59E-05</th><th>7.14E-05</th><th>8.70E-05</th><th>1.03E-04</th><th>1.85E-04</th><th>3.41E-04</th><th>8.09E-04</th><th>1.59E-03</th></td<>	<sup>223</sup> Ra	$\alpha, \gamma$	11.435 days	4.00E-05	5.59E-05	7.14E-05	8.70E-05	1.03E-04	1.85E-04	3.41E-04	8.09E-04	1.59E-03
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	<sup>224</sup> Ra	$\alpha, \gamma$	3.66 days	7.81E-03	2.89E-03	1.07E-03	3.98E-04	1.48E-04	1.91E-06	8.94E-07	9.08E-07	9.37E-07
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	<sup>87</sup> Rb	$\beta^-$	4.88×10 <sup>10</sup> years	1.39E-05	1.39E-05	1.39E-05	1.39E-05	1.39E-05	1.39E-05	1.39E-05	1.39E-05	1.39E-05
β <sup>+</sup> , γ         29.9 seconds         0.00E+00	<sup>102</sup> Rh	$\beta^-$ , $\gamma$ , $\epsilon\beta^+$	207 days	1.26E-13	5.26E-24	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
$\alpha$ , $\gamma$ 3.96 seconds4.00E-055.59E-057.14E-058.70E-051.03E-041.85E-041.85E-043.41E-04 $\alpha$ , $\gamma$ 55.6 seconds7.81E-032.89E-031.07E-033.98E-041.48E-041.91E-068.94E-07 $\beta^{-}$ 1.02 years0.00E+000.00E+000.00E+000.00E+000.00E+000.00E+00 $\beta^{-}$ 2.758 years9.11E-118.53E-220.00E+000.00E+000.00E+000.00E+00 $\beta^{-}$ 1.2.4 days5.39E-025.38E-025.38E-025.37E-025.3E-02 $\beta^{-}$ 1.2.4 days3.85E-013.84E-013.84E-013.84E-013.82E-01 $\beta^{-}$ $\beta^{-}$ 1.128 days3.51E-024.57E-024.57E-024.56E-024.56E-02 $\beta^{-}$ $\beta^{-}$ 1.128 days3.51E-013.64E-023.0E-032.27E-034.16E-061.40E-11 $\beta^{-}$ $\beta^{-}$ 1.0×10 <sup>5</sup> years3.85E-013.84E-013.84E-013.84E-013.84E-013.84E-01 $\beta^{-}$	106Rh	β <sup>-</sup> , γ	29.9 seconds	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
$\alpha$ , $\gamma$ $55.6$ seconds $7.81E-03$ $2.89E-03$ $1.07E-03$ $3.98E-04$ $1.48E-04$ $1.91E-06$ $8.94E-07$ $\beta^{+}$ $1.02$ years $0.00E+00$ $0.00E+00$ $0.00E+00$ $0.00E+00$ $0.00E+00$ $0.00E+00$ $0.00E+00$ $0.00E+00$ $\beta^{+}$ , $\gamma$ $2.758$ years $9.11E-11$ $8.53E-22$ $0.00E+00$ $0.00E+00$ $0.00E+00$ $0.00E+00$ $0.00E+00$ $0.00E+00$ $\beta^{+}$ , $\gamma$ $12.4$ days $5.39E-02$ $5.38E-02$ $5.38E-02$ $5.38E-02$ $5.38E-02$ $5.38E-02$ $5.38E-02$ $5.38E-02$ $5.38E-02$ $\beta^{+}$ $\gamma$ $12.4$ days $3.85E-01$ $3.85E-01$ $3.84E-01$ $3.84E-01$ $3.84E-01$ $3.84E-01$ $3.84E-01$ $3.84E-01$ $3.84E-01$ $3.84E-01$ $3.84E-01$ $3.84E-02$ $4.56E-02$ <t< th=""><th><sup>219</sup>Rn</th><th><math>\alpha, \gamma</math></th><th>3.96 seconds</th><th>4.00E-05</th><th>5.59E-05</th><th>7.14E-05</th><th>8.70E-05</th><th>1.03E-04</th><th>1.85E-04</th><th>3.41E-04</th><th>8.09E-04</th><th>1.59E-03</th></t<>	<sup>219</sup> Rn	$\alpha, \gamma$	3.96 seconds	4.00E-05	5.59E-05	7.14E-05	8.70E-05	1.03E-04	1.85E-04	3.41E-04	8.09E-04	1.59E-03
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	<sup>220</sup> Rn	$\alpha, \gamma$	55.6 seconds	7.81E-03	2.89E-03	1.07E-03	3.98E-04	1.48E-04	1.91E-06	8.94E-07	9.08E-07	9.37E-07
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	106Ru	$\beta^-$	1.02 years	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	125Sb	$\beta^-$ , $\gamma$	2.758 years	9.11E-11	8.53E-22	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	126Sb	$\beta^-, \gamma$	12.4 days	5.39E-02	5.38E-02	5.38E-02	5.38E-02	5.37E-02	5.35E-02	5.32E-02	5.21E-02	5.03E-02
$ \begin{array}{ c c c c c c c c c c c c c c c c c c c$	126mSb	$\gamma, ITe^-$	11 seconds	3.85E-01	3.85E-01	3.84E-01	3.84E-01	3.84E-01	3.82E-01	3.80E-01	3.72E-01	3.59E-01
n $\beta$ , $\gamma$ 90 years         9.75E+01         4.51E+01         2.09E+01         9.67E+00         4.48E+00         9.52E-02         4.30E-05           n $\beta$ -         1.128 days         3.51E-01         9.95E-02         2.82E-02         8.00E-03         2.27E-03         4.16E-06         1.40E-11           sn $\beta$ -, $\gamma$ , $IZe$ -         55 years         4.52E-01         1.28E-01         3.84E-01         3.84E-01         3.84E-01         3.84E-01         3.84E-01         3.84E-01         3.84E-01         4.48E-07         1.11E-17	eS <sub>62</sub>	$\beta^-$	6.5×10 <sup>4</sup> years	4.57E-02	4.57E-02	4.57E-02	4.57E-02	4.56E-02	4.56E-02	4.55E-02	4.52E-02	4.47E-02
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	<sup>151</sup> Sm	$\beta^-, \gamma$	90 years	9.75E+01	4.51E+01	2.09E+01	9.67E+00	4.48E+00	9.52E-02	4.30E-05	3.96E-15	6.85E-32
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	<sup>121</sup> Sn	β_	1.128 days	3.51E-01	9.95E-02	2.82E-02	8.00E-03	2.27E-03	4.16E-06	1.40E-11	5.36E-28	0.00E+00
$\beta, \gamma$ 1.0×10 <sup>5</sup> years 3.85E-01 3.84E-01 3.84E-01 3.84E-01 3.84E-01 3.84E-01 3.82E-01 3.80E-01 3.80E-01 3.11E-17	121mSn	$\beta^-$ , $\gamma$ , $ITe^-$	55 years	4.52E-01	1.28E-01	3.64E-02	1.03E-02	2.92E-03	5.36E-06	1.81E-11	6.90E-28	0.00E+00
B	126Sn	β <sup>-</sup> , γ	1.0×10 <sup>5</sup> years	3.85E-01	3.85E-01	3.84E-01	3.84E-01	3.84E-01	3.82E-01	3.80E-01	3.72E-01	3.59E-01
	3S <sub>06</sub>	β_	29.1 years	2.32E+03	1.97E+02	1.68E+01	1.43E+00	1.22E-01	5.48E-07	1.11E-17	0.00E+00	0.00E+00

IV-4 of IV-10

ANL-WIS-MD-000009 REV 01

Table IV-1. Yucca Mountain Project Radionuclide Inventory for Pressurized-Water Reactor Fuels (Continued)

Nuclide	Decay	(q) 3: 1 31-11				Radioactivity	Radioactivity Inventory [Ci/Assembly]	:i/Assembly]			
Q	$Mode^{(a)}$	нап-спе	125 yr	225 yr	325 yr	425 yr	525 yr	1,025 yr	2,025 yr	5,025 yr	10,025 yr
э1 <sub>66</sub>	β <sup>-</sup> , γ	2.13×10 <sup>5</sup> years	8.98E+00	8.98E+00	8.98E+00	8.97E+00	8.97E+00	8.96E+00	8.93E+00	8.84E+00	8.69E+00
<sup>125m</sup> Te	$\gamma,\ ITe^-$	58 days	2.23E-11	2.08E-22	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
<sup>227</sup> Th	$\alpha, \beta^-, \gamma$	18.72 days	3.95E-05	5.51E-05	7.05E-05	8.58E-05	1.01E-04	1.83E-04	3.36E-04	7.98E-04	1.57E-03
<sup>228</sup> Th	$\alpha, \gamma$	1.913 years	7.81E-03	2.89E-03	1.07E-03	3.98E-04	1.48E-04	1.91E-06	8.94E-07	9.08E-07	9.37E-07
<sup>230</sup> Th	$\alpha, \beta^-, \gamma$	7.54×10 <sup>4</sup> years	1.00E-03	2.14E-03	3.40E-03	4.73E-03	6.08E-03	1.29E-02	2.64E-02	6.61E-02	1.29E-01
<sup>231</sup> Th	$\beta^-, \gamma$	1.063 days	7.38E-03	7.40E-03	7.42E-03	7.43E+00	7.45E-03	7.54E-03	7.71E-03	8.19E-03	8.91E-03
<sup>234</sup> Th	$\beta^-, \gamma$	24.10 days	1.48E-01	1.48E-01	1.48E-01	1.48E-01	1.48E-01	1.48E-01	1.48E-01	1.48E-01	1.48E-01
11 <sub>202</sub>	β_	4.77 minutes	3.99E-05	5.57E-05	7.12E-05	8.67E-05	1.02E-04	1.85E-04	3.40E-04	8.07E-04	1.58E-03
11 <sub>802</sub>	β_	3.053 minutes	2.81E-03	1.04E-03	3.85E-04	1.43E-04	5.32E-05	6.86E-07	3.21E-07	3.26E-07	3.37E-07
<sub>232</sub> U	α	70 years	7.59E-03	2.81E-03	1.04E-03	3.87E-04	1.44E-04	1.87E-06	8.76E-07	8.60E-07	8.35E-07
<sub>233</sub> U	α	1.592×10 <sup>5</sup> years	1.62E-04	3.21E-04	5.08E-04	7.19E-04	9.52E-04	2.33E-03	5.61E-03	1.60E-02	3.32E-02
<sup>234</sup> U	α	2.46×10 <sup>5</sup> years	1.12E+00	1.33E+00	1.42E+00	1.46E+00	1.48E+00	1.49E+00	1.49E+00	1.48E+00	1.46E+00
<sup>235</sup> U	α	7.04×10 <sup>8</sup> years	7.38E-03	7.40E-03	7.42E-03	7.43E-03	7.45E-03	7.54E-03	7.71E-03	8.19E-03	8.91E-03
<sub>236</sub> U	α	2.342×10 <sup>7</sup> years	1.73E-01	1.74E-01	1.74E-01	1.75E-01	1.76E-01	1.81E-01	1.89E-01	2.09E-01	2.30E-01
<sub>237</sub> U	β_	6.75 days	4.71E-03	4.48E-05	7.46E-06	7.11E-06	7.05E-06	6.77E-06	6.24E-06	4.88E-06	3.25E-06
<sub>238</sub> U	α	4.47×10 <sup>9</sup> years	1.48E-01	1.48E-01	1.48E-01	1.48E-01	1.48E-01	1.48E-01	1.48E-01	1.48E-01	1.48E-01
$\lambda_{06}$	β_	2.67 days	2.32E+03	1.97E+02	1.68E+01	1.43E+00	1.22E-01	5.48E-07	1.11E-17	0.00E+00	0.00E+00
<sub>93</sub> Zr	β_	1.5×10 <sup>6</sup> years	8.94E-01	8.94E-01	8.94E-01	8.94E-01	8.94E-01	8.94E-01	8.93E-01	8.92E-01	8.90E-01
		Total <sup>(c)</sup> =	1.70E+04	4.38E+03	2.69E+03	2.18E+03	1.87E+03	1.09E+03	6.03E+02	3.95E+02	2.86E+02

Source: CRWMS M&O 1999 [DIRS 136429] Attachment X

NOTES: <sup>a</sup> Decay modes identified from Parrington et al. (1996 [DIRS 103896]).
<sup>b</sup> Half-lives identified from Parrington et al. (1996 [DIRS 103896]).
<sup>c</sup> Total radionuclide activities are calculated here and are not part of original reference.

Decay times listed in Table IV-1 include the 25-year decay time of the fuels prior to its emplacement into the YMP repository. Thus, fuel with a date of 525 years corresponds to fuel that has been stored for 500 years (calendar year 2535) in the repository.

Table IV-2. Yucca Mountain Project Radionuclide Inventory for Boiling-Water Reactor Fuels

							1				
Nuclide	Decay Mode(a)	(q) °9!   3 °11	406	177	206	Nauloaciivii 425 :::	And the first of t	4 one		200	40.005
108 4 2	+0- : -0	nair-Life"	125 yr	225 yr	325 yr	425 yr	525 yr	1,025 yr	2,025 yr	5,025 yr	10,025 yr
AG	дз , Х , с	Z.39III	1.93E-04	1.1ZE-04	0.40E-U3	3.70E-U3	Z. IOE-U3	1.42E-U0	0.00E-03	4.00E-10	0.39E-20
108mAg	$\gamma$ , $\epsilon \beta^+$ , $ITe^-$	130 years	2.22E-03	1.29E-03	7.46E-04	4.32E-04	2.50E-04	1.63E-05	6.96E-08	5.39E-15	7.58E-27
<sup>241</sup> Am	$\alpha, \gamma, SF$	432.7 years	6.72E+02	5.74E+02	4.89E+02	4.17E+02	3.55E+02	1.59E+02	3.21E+01	2.90E-01	1.80E-02
<sup>242</sup> Am	$\beta^-$ , $\gamma$ , $\epsilon e^-$	16.02 hours	1.32E+00	8.07E-01	4.94E-01	3.02E-01	1.85E-01	1.58E-02	1.16E-04	4.56E-11	9.64E-22
<sup>242m</sup> Am	$\alpha, \gamma, ITe^-, SF$	141 years	1.33E+00	8.10E-01	4.96E-01	3.03E-01	1.85E-01	1.59E-02	1.16E-04	4.58E-11	9.69E-22
<sup>243</sup> Am	$\alpha, \gamma, SF$	7370 years	5.29E+00	5.24E+00	5.19E+00	5.14E+00	5.09E+00	4.86E+00	4.42E+00	3.34E+00	2.08E+00
39Ar	$\beta^-$	269 years	1.24E-05	9.59E-06	7.41E-06	5.73E-06	4.43E-06	1.22E-06	9.28E-08	4.07E-11	1.03E-16
137mBa	IT	2.552 minutes	1.30E+03	1.29E+02	1.28E+01	1.27E+00	1.26E-01	1.21E-06	1.11E-16	0.00E+00	0.00E+00
<sup>212</sup> Bi	$\alpha, \beta^-, \gamma$	1.009 hours	1.77E-03	6.55E-04	2.43E-04	9.01E-05	3.35E-05	3.98E-07	1.69E-07	1.77E-07	1.92E-07
14C	$\beta^-$	5730 years	1.73E-01	1.71E-01	1.69E-01	1.67E-01	1.65E-01	1.56E-01	1.38E-01	9.59E-02	5.24E-02
<sup>41</sup> Ca	သ	1.03×10 <sup>5</sup> years	3.73E-05	3.72E-05	3.72E-05	3.72E-05	3.72E-05	3.70E-05	3.68E-05	3.60E-05	3.49E-05
113mCd	$\beta^-$ , IT	14.1 years	1.66E-02	1.22E-04	8.91E-07	6.53E-09	4.79E-11	1.01E-21	0.00E+00	0.00E+00	0.00E+00
<sup>144</sup> Ce	$\beta^-, \gamma$	284.6 days	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3 <sub>9</sub> Cl	$\beta^-,  \beta^+,  \epsilon$	3.01×10 <sup>5</sup> years	2.93E-03	2.93E-03	2.93E-03	2.93E-03	2.93E-03	2.92E-03	2.92E-03	2.90E+00	2.86E+00
<sup>242</sup> Cm	$\alpha, \gamma, SF$	1.2×10 <sup>3</sup> years	1.09E+00	6.67E-01	4.08E-01	2.50E-01	1.53E-01	1.31E-02	9.58E-05	3.78E-11	8.00E-22
<sup>243</sup> Cm	$\alpha, \gamma, SF, \varepsilon$	162.8 days	2.17E-01	1.91E-02	1.68E-03	1.47E-04	1.29E-05	6.76E-11	1.85E-21	0.00E+00	0.00E+00
<sup>244</sup> Cm	$\alpha, \gamma, SF$	29.1 years	5.54E+00	1.20E-01	2.61E-03	5.67E-05	1.23E-06	5.94E-15	1.37E-31	0.00E+00	0.00E+00
<sup>245</sup> Cm	$\alpha, \gamma, SF$	18.1 years	4.00E-02	3.97E-02	3.93E-02	3.90E-02	3.87E-02	3.71E-02	3.42E-02	2.68E-02	1.78E-02
<sup>246</sup> Cm	$\alpha, \gamma, SF$	8.5×10 <sup>3</sup> years	1.43E-02	1.41E-02	1.39E-02	1.37E-02	1.35E-02	1.25E-02	1.08E-02	6.97E-03	3.35E-03
°00	β <sup>-</sup> , γ	4.76×10 <sup>3</sup> years	8.51E-05	1.65E-10	3.19E-16	6.18E-22	1.20E-27	0.00E+00	0.00E+00	0.00E+00	0.00E+00
134Cs	β <sup>-</sup> , γ,ε	5.271 years	1.59E-14	3.98E-29	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
135Cs	$\beta^-$	2.065 years	1.39E-01	1.39E-01	1.39E-01	1.39E-01	1.39E-01	1.39E-01	1.39E-01	1.39E-01	1.38E-01
<sup>137</sup> Cs	β <sup>-</sup> , γ	2.3×10 <sup>6</sup> years	1.37E+03	1.36E+02	1.35E+01	1.34E+00	1.33E-01	1.28E-06	1.18E-16	0.00E+00	0.00E+00
<sup>152</sup> Eu	$\beta^-, \gamma, \epsilon \beta^+$	13.48 years	2.92E-03	1.61E-05	8.86E-08	4.88E-10	2.69E-12	1.37E-23	0.00E+00	0.00E+00	0.00E+00
<sup>154</sup> Eu	$\beta^-, \gamma, \epsilon \gamma$	8.59 years	5.45E-02	1.71E-05	5.34E-09	1.68E-12	5.23E-16	0.00E+00	0.00E+00	0.00E+00	0.00E+00
<sup>155</sup> Eu	β <sup>-</sup> , γ	4.71 years	5.91E-06	2.19E-12	8.07E-19	2.98E-25	1.14E-31	0.00E+00	0.00E+00	0.00E+00	0.00E+00
<sub>55</sub> Fе	3	2.73 years	1.02E-11	9.56E-23	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
<b>Н</b> <sub>е</sub>	$\beta^-$	12.3 years	1.43E-01	5.17E-04	1.87E-06	6.75E-09	2.45E-11	1.51E-23	0.00E+00	0.00E+00	0.00E+00
166mHo	$\beta^-, \gamma$	1.2×10 <sup>3</sup> years	1.11E-03	1.05E-03	9.93E-04	9.37E-04	8.84E-04	6.62E-04	3.72E-04	6.58E-05	3.66E-06

IV-6 of IV-10

ANL-WIS-MD-000009 REV 01

Table IV-2. Yucca Mountain Project Radionuclide Inventory for Boiling-Water Reactor Fuels (Continued)

Nuclide	Decav					Radioactivi	Radioactivity Inventory [Ci/Assembly]	Ci/Assembly			
<b>Q</b>	Mode <sup>(a)</sup>	Half-Life <sup>(b)</sup>	125 yr	225 yr	325 yr	425 yr	525 yr	1,025 yr	2,025 yr	5,025 yr	10,025 yr
129 <sub>1</sub>	$\beta^-, \gamma$	1.57×10 <sup>7</sup> years	7.42E-03	7.42E-03	7.42E-03	7.42E-03	7.42E-03	7.42E-03	7.42E-03	7.42E-03	7.42E-03
85Kr	$\beta^-, \gamma$	10.73 years	5.93E-01	9.21E-04	1.43E-06	2.23E-09	3.46E-12	3.15E-26	0.00E+00	0.00E+00	0.00E+00
<sub>93</sub> Mo	$\gamma,  \epsilon,  e^-$	~3.5×10³ years	2.17E-04	2.13E-04	2.09E-04	2.05E-04	2.01E-04	1.82E-04	1.49E-04	8.24E-05	3.06E-05
qN <sub>wE6</sub>	ITe-	16.1 years	3.41E-01	3.39E-01	3.39E-01	3.39E-01	3.39E-01	3.39E-01	3.38E-01	3.38E-01	3.36E-01
<sub>94</sub> Nb	β <sup>-</sup> , γ	2.0×10 <sup>4</sup> years	1.86E-02	1.86E-02	1.85E-02	1.84E-02	1.84E-02	1.81E-02	1.75E-02	1.58E-02	1.33E-02
iN <sub>69</sub>	ω	7.6×10 <sup>4</sup> years	5.02E-01	5.01E-01	5.01E-01	5.00E-01	5.00E-01	4.97E-01	4.93E-01	4.79E-01	4.58E-01
<sup>63</sup> Ni	β_	100 years	2.93E+01	1.47E+01	7.34E+00	3.67E+00	1.84E+00	5.76E-02	5.66E-05	5.38E-14	4.94E-29
<sup>237</sup> Np	$\alpha, \gamma$	2.14×10 <sup>6</sup> years	9.09E-02	1.11E-01	1.28E-01	1.43E-01	1.55E-01	1.95E-01	2.21E-01	2.27E-01	2.26E-01
<sup>238</sup> Np	$\beta^-, \gamma$	2.117 days	5.96E-03	3.65E-03	2.23E-03	1.36E-03	8.35E-04	7.15E-05	5.24E-07	2.06E-13	4.36E-24
dN <sup>652</sup>	$\beta^-, \gamma, SF$	1.2×10 <sup>4</sup> years	5.29E+00	5.24E+00	5.19E+00	5.14E+00	5.09E+00	4.86E+00	4.42E+00	3.34E+00	2.08E+00
<sup>231</sup> Pa	$\alpha, \gamma$	3.28×10 <sup>4</sup> years	1.95E-05	2.50E-05	3.05E-05	3.60E-05	4.15E-05	6.91E-05	1.24E-04	2.89E-04	5.59E-04
<sup>233</sup> Pa	$\beta^-, \gamma$	27.0 days	9.09E-02	1.11E-01	1.28E-01	1.43E-01	1.55E-01	1.95E-01	2.21E-01	2.27E-01	2.26E-01
<sup>234</sup> Pa	β <sup>-</sup> , γ	6.69 hours	8.21E-05	8.21E-05	8.21E-05	8.21E-05	8.21E-05	8.21E-05	8.21E-05	8.21E-05	8.21E-05
<sup>234m</sup> Pa	$\beta^-, \gamma, IT$	1.17 minutes	6.32E-02	6.32E-02	6.32E-02	6.32E-02	6.32E-02	6.32E-02	6.32E-02	6.32E-02	6.32E-02
<sup>212</sup> Pb	β <sup>-</sup> , γ	10.64 hours	1.77E-03	6.55E-04	2.43E-04	9.01E-05	3.35E-05	3.98E-07	1.69E-07	1.77E-07	1.92E-07
<sup>107</sup> Pd	β_	6.5×10 <sup>6</sup> years	2.65E-02	2.65E-02	2.65E-02	2.65E-02	2.65E-02	2.65E-02	2.65E-02	2.65E-02	2.65E-02
<sup>145</sup> Pm	α, γ, ε	17.7 years	5.20E-06	1.03E-07	2.06E-09	4.10E-11	8.18E-13	2.56E-21	0.00E+00	0.00E+00	0.00E+00
<sup>146</sup> Pm	$\beta^-, \gamma, \epsilon \gamma$	5.53 years	8.95E-08	3.22E-13	1.16E-18	4.16E-24	1.49E-29	0.00E+00	0.00E+00	0.00E+00	0.00E+00
<sup>147</sup> Pm	β <sup>-</sup> , γ	2.6234 years	1.33E-10	4.45E-22	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
<sup>212</sup> Po	α	0.298 ms	1.13E-03	4.20E-04	1.56E-04	5.77E-05	2.14E-05	2.55E-07	1.08E-07	1.13E-07	1.23E-07
<sup>216</sup> Po	α, γ	0.145 seconds	1.77E-03	6.55E-04	2.43E-04	9.01E-05	3.35E-05	3.98E-07	1.69E-07	1.77E-07	1.92E-07
<sup>144</sup> Pr	β <sup>-</sup> , γ	17.28 minutes	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
<sub>236</sub> Pu	$\alpha, \gamma, SF$	2.87 years	1.64E-07	1.64E-07	1.64E-07	1.64E-07	1.64E-07	1.63E-07	1.62E-07	1.59E-07	1.55E-07
<sub>238</sub> Pu	$\alpha, \gamma, SF$	87.7 years	2.66E+02	1.21E+02	5.53E+01	2.52E+01	1.16E+01	2.49E-01	1.88E-04	1.01E-10	2.13E-21
<sub>239</sub> Pu	$\alpha, \gamma, SF$	2.410×10 <sup>4</sup>	5.33E+01	5.32E+01	5.31E+01	5.29E+01	5.28E+01	5.21E+01	5.08E+01	4.69E+01	4.10E+01
<sup>240</sup> Pu	$\alpha, \gamma, SF$	$6.56 \times 10^{3}$	1.13E+02	1.12E+02	1.11E+02	1.10E+02	1.09E+02	1.03E+02	9.28E+01	6.76E+01	3.98E+01
<sup>241</sup> Pu	$\alpha, \beta^-, \gamma$	14.4 years	5.41E+01	4.71E-01	4.28E-02	3.91E-02	3.88E-02	3.72E-02	3.43E-02	2.69E-02	1.79E-02
<sup>242</sup> Pu	$\alpha, \gamma, SF$	3.75×10 <sup>5</sup> years	5.08E-01	5.08E-01	5.08E-01	5.08E-01	5.08E-01	5.07E-01	5.06E-01	5.04E-01	4.99E-01
<sup>224</sup> Ra	$\alpha, \gamma$	3.66 days	1.77E-03	6.55E-04	2.43E-04	9.01E-05	3.35E-05	3.98E-07	1.69E-07	1.77E-07	1.92E-07
<sup>102</sup> Rh	$\beta^-, \gamma, \epsilon \beta^+$	207 days	2.72E-14	1.13E-24	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
<sup>106</sup> Rh	β <sup>-</sup> , γ	29.9 seconds	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00

IV-7 of IV-10

ANL-WIS-MD-000009 REV 01

Table IV-2. Yucca Mountain Project Radionuclide Inventory for Boiling-Water Reactor Fuels (Continued)

Alclide	Decay					Radioactivit	y Inventory [	Radioactivity Inventory [Ci/Assembly]			
ID	Mode <sup>(a)</sup>	Half-Life <sup>(b)</sup>	125 yr	225 yr	325 yr	425 yr	525 yr	1,025 yr	2,025 yr	5,025 yr	10,025 yr
<sup>220</sup> Rn	$\alpha, \gamma$	55.6 seconds	1.77E-03	6.55E-04	2.43E-04	9.01E-05	3.35E-05	3.98E-07	1.69E-07	1.77E-07	1.92E-07
<sup>106</sup> Ru	β_	1.02 years	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
<sup>125</sup> Sb	$\beta^-, \gamma$	2.758 years	2.71E-11	2.54E-22	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
126Sb	$\beta^-, \gamma$	12.4 days	1.77E-02	1.77E-02	1.77E-02	1.77E-02	1.77E-02	1.76E-02	1.75E-02	1.71E-02	1.66E-02
126mSb	$\gamma, ITe^-$	11 seconds	1.27E-01	1.27E-01	1.26E-01	1.26E-01	1.26E-01	1.26E-01	1.25E-01	1.22E-01	1.18E-01
29Se	β_	6.5×10 <sup>4</sup> years	1.59E-02	1.59E-02	1.59E-02	1.59E-02	1.59E-02	1.59E-02	1.58E-02	1.57E-02	1.56E-02
151Sm	$\beta^-, \gamma$	90 years	2.50E+01	1.16E+01	5.35E+00	2.48E+00	1.15E+00	2.43E-02	1.10E-05	1.01E-15	2.28E-32
<sup>121</sup> Sn	β_	1.128 days	1.32E-01	3.74E-02	1.06E-02	3.00E-03	8.52E-04	1.56E-06	5.27E-12	2.01E-28	0.00E+00
121mSn	$\beta^-, \gamma, ITe^-$	55 years	1.70E-01	4.81E-02	1.37E-02	3.87E-03	1.10E-03	2.02E-06	6.78E-12	2.59E-28	0.00E+00
<sup>126</sup> Sn	$\beta^-, \gamma$	1.0×10 <sup>5</sup> years	1.27E-01	1.27E-01	1.26E-01	1.26E-01	1.26E-01	1.26E-01	1.25E-01	1.22E-01	1.18E-01
oSr	β_	29.1 years	8.13E+02	6.92E+01	5.90E+00	5.03E-01	4.28E-02	1.92E-07	3.88E-18	0.00E+00	0.00E+00
<sub>99</sub> Tc	$\beta^-$ , $\gamma$	2.13×10 <sup>5</sup> years	3.20E+00	3.20E+00	3.20E+00	3.20E+00	3.20E+00	3.19E+00	3.18E+00	3.15E+00	3.10E+00
<sup>125m</sup> Te	$\gamma, ITe^-$	58 days	6.61E-12	6.21E-23	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
<sup>228</sup> Th	$\alpha, \gamma$	1.913 years	1.77E-03	6.55E-04	2.43E-04	9.01E-05	3.35E-05	3.98E-07	1.69E-07	1.77E-07	1.92E-07
<sup>230</sup> Th	$\alpha, \gamma$	7.54×10 <sup>4</sup> years	3.49E-04	7.10E-04	1.10E-03	1.51E-03	1.93E-03	4.02E-03	8.17E-03	2.03E-02	3.97E-02
<sup>231</sup> Th	$\beta^-, \gamma$	1.063 days	2.63E-03	2.63E-03	2.64E-03	2.64E-03	2.65E-03	2.68E-03	2.73E-03	2.87E-03	3.09E-03
<sup>234</sup> Th	$\beta^-, \gamma$	24.10 days	6.32E-02	6.32E-02	6.32E-02	6.32E-02	6.32E-02	6.32E-02	6.32E-02	6.32E-02	6.32E-02
208 11	$\beta^-, \gamma$	3.053 minutes	6.35E-04	2.35E-04	8.73E-05	3.24E-05	1.20E-05	1.43E-07	6.06E-08	6.34E-08	6.88E-08
<sub>232</sub> U	$\alpha, \gamma, SF$	70 years	1.72E-03	6.37E-04	2.36E-04	8.76E-05	3.25E-05	3.88E-07	1.62E-07	1.59E-07	1.55E-07
<sub>233</sub> U	$\alpha, \gamma, SF$	1.592×10 <sup>5</sup> years	4.53E-05	8.94E-05	1.42E-04	2.01E-04	2.66E-04	6.51E-04	1.57E-03	4.47E-03	9.26E-03
<sup>234</sup> U	$\alpha, \gamma, SF$	2.46×10 <sup>5</sup> years	3.64E-01	4.16E-01	4.39E-01	4.50E-01	4.55E-01	4.58E-01	4.57E-01	4.54E-01	4.48E-01
<sup>235</sup> U	$\alpha, \gamma, SF$	7.04×10 <sup>8</sup> years	2.63E-03	2.63E-03	2.64E-03	2.64E-03	2.65E-03	2.68E-03	2.73E-03	2.87E-03	3.09E-03
<sub>236</sub> U	$\alpha, \gamma, SF$	2.342×10 <sup>7</sup> years	6.30E-02	6.33E-02	6.36E-02	6.39E-02	6.43E-02	6.58E-02	6.87E-02	7.58E-02	8.35E-02
		Total <sup>(c)</sup> =	4.72E+03	1.24E+03	7.71E+02	6.32E+02	5.49E+02	3.31E+02	1.91E+02	1.28E+02	9.15E+01

Source: CRWMS M&O 1999 [DIRS 136429] Attachment X

NOTES: <sup>a</sup> Decay modes identified from Parrington et al. (1996 [DIRS 103896]).
<sup>b</sup> Half-lives identified from Parrington et al. (1996 [DIRS 103896]).
<sup>c</sup> Total radionuclide activities are calculated here and are not part of original reference.

Decay times listed in Table IV-2 include the 25-year decay time of the fuels prior to its emplacement into the YMP repository. Thus, fuel with a date of 525 years corresponds to fuel that has been stored for 500 years (calendar year 2535) in the repository.

ANL-WIS-MD-000009 REV 01

Table IV-3. Alpha Recoil Enhanced (from Both  $\alpha$  and  $\alpha$ -Recoil Atom) Dissolution Rates Due to the Major Mass-Based Constituents of SNF and HLW to be Disposed in the Yucca Mountain Repository

Nuclide ID	Decay Mode	Half–Life <sup>(a)</sup> (yr)	Fraction Decay Rate <sup>(b)</sup> (1/yr)	α–Decay Rate in 13 Mono-Layers <sup>(c)</sup> (g/m²–yr)
<sup>238</sup> U	α, γ, SF	4.47 x 10 <sup>9</sup>	1.55 x 10 <sup>-10</sup>	6.05 x 10 <sup>-12</sup>
<sup>235</sup> U	α, γ, SF	7.04 x 10 <sup>8</sup>	9.85 x 10 <sup>-10</sup>	3.84 x 10 <sup>-11</sup>
<sup>239</sup> Pu	α, γ, SF	2.410 x 10 <sup>4</sup>	2.88 x 10 <sup>-5</sup>	1.12 x 10 <sup>-6</sup>
<sup>236</sup> U	α, γ, SF	2.342 x 10 <sup>7</sup>	2.96 x 10 <sup>-8</sup>	1.15 x 10 <sup>-9</sup>

NOTES: <sup>a</sup> Half-life values in Sanchez et al. (1998 [DIRS 149368]).

<sup>b</sup> The fraction decay rate, also known as the decay constant, is given by  $\lambda = \ln(2)/\iota \frac{1}{2}$ , where  $\iota \frac{1}{2}$  is the radionuclide half-life given by values in column 3.

<sup>c</sup> Each mono-layer thickness is 3.0 Å (3.0x10-10m), and the density is upper bounded at 19.86 g/cm3 (theoretical density of pure plutonium metal) (Wick 1980 [DIRS 143651]).

INTENTIONALLY LEFT BLANK

# ATTACHMENT V - DATA QUALIFICATION FOR DIRECT INPUTS TO MISCELLANEOUS WASTE-FORM FEPS

This attachment is related to the miscellaneous waste-form FEPs as discussed in Section 6.2. This attachment provides the results of data qualification activities for previously unqualified project data and documents per the data qualification tasks as required by AP-SIII.2Q, *Qualification of Unqualified Data*, and for data obtained from outside sources that are not "established fact" per the requirements found in AP-SIII.9Q, *Scientific Analyses*. It is not intended as stand-alone documentation separate from the main document. The data qualified herein is intended for use only for FEPs screening and, more specifically, for use within this work product. The data qualification activity was detailed in the qualification plan (Attachment VI).

The miscellaneous waste-form FEPs analyses require the use of input, cited from journal papers, compendiums, proceedings, internet citations, and other sources, to represent the nature, magnitude, and potential consequence of the miscellaneous waste-form FEPs. The use and classification of such input is subject to classification per Attachment 3 of AP-3.15Q, Managing Technical Product Inputs, because the information satisfies the definition of "direct input." Project-generated information directly used in the analysis is identified as data because it is the "result of activities such as sample collection, physical measurements, testing, and analysis, both in the field and in the laboratory, that are not site-specific and do not meet the definition of Established Fact." Because this "data" does not initially satisfy the definition in Attachment 3 as "qualified," it is thus subject to the requirements of AP-SIII.2Q, which allows data qualification to be conducted within the work product, so long as 1) the qualification is "providing a desired level of confidence that the data are suitable for their intended use" and 2) "the intended use the data is only for that work product." For "data" obtained from outside sources that are not established facts, the requirements identified in AP-SIII.9Q are used to qualify the data for use within the technical product (i.e., this analysis report). Given these conditions, then no action is required under AP-3.15Q, Managing Technical Product Inputs. The direct input qualified here, along with the direct input from YMP-controlled sources, is listed in Section 4 per requirements of AP-SIII.9Q, Scientific Analyses.

The information sources in this attachment are to be qualified in accordance with Attachment 3 of AP-SIII.2Q, *Qualification of Unqualified Data*, which states:

The Data Qualification Report includes, as applicable, a discussion of the following items:

- 1. The data set(s) for qualification
- 2. The method(s) of qualification selected and rationale
- 3. Evaluation criteria
- 4. An evaluation of the technical correctness of the data, as applicable
- 5. Data generated by the evaluation, if applicable

- 6. The evaluation results
- 7. A conclusion for/against changing the qualification status of the data based on the team's judgments in response to the evaluation criteria and the evaluation results. Refer to the Technical Work Plan or Attachment 2, Data Qualification Plan, as appropriate.
- 8. The rationale for abandoning any of the qualification methods, if appropriate
- 9. A discussion of any limits or caveats that should be considered by potential users of the data
- 10. Identification of any supporting information used in the qualification effort by the appropriate reference identifier (Data Tracking Number [DTN], accession number, Technical Information Center catalog number, etc.)
- 11. Reference to the Technical Work Plan or Attachment 2, Data Qualification Plan. Deviations to the plan should be documented and justified in the report.

Additionally, the non-project sources of information in this report are to be qualified in accordance with AP-SIII.9Q, Scientific Analyses, (Rev. 1/ICN 4, Section 5.2.1(l)) which uses the following factors in qualifying data as suitable for its intended use:

- Reliability of data source.
- Qualification of personnel or organizations.
- Extent to which the data demonstrate the properties of interest.
- Prior uses of the data.
- Availability of corroborating data.

This attachment has been organized in accordance with the above list of data qualification items. Each item listed above is given an individual section. Accordingly, Section 4 provides the evaluation of the data, and contains the discussion wherein the direct inputs are corroborated.

# V.1 DATA SOURCES FOR QUALIFICATION

The direct inputs requiring qualification for use in this analysis report were identified in the Data Qualification Plan (Attachment VI) and are shown in Table V-1. Subsequent to the development of the initial plan, *FEPs Screening of Processes and Issues in Drip Shield and Waste Package Degradation* (BSC 2004 [DIRS 162200]) was identified as a more appropriate direct input source to Section 6.2.37 than the reference previously used (CRWMS M&O 1997 [DIRS 100264]). Accordingly, there was no need to qualify *Waste Package Design Basis Events* (CRWMS M&O 1997 [DIRS 100264]) in this data qualification report.

Each of the remaining three sources to be qualified is identified by the section used in the report and FEP number, and will be treated separately within Section V.4. Table V-2 also addresses the corroborating information used in the FEPs screening arguments (for excluded FEPs) and TSPA disposition descriptions (for included FEPs) in Section 6.2 of this document (currently, all three of the direct inputs to be qualified are used in screening arguments for excluded FEPs).

The source column in Table V-1 provides the citation as it appears in the DIRS database and provides traceability through the TIC number or DIRS numbers as required by AP-SIII.2Q, *Qualification of Unqualified Data*. The description column in the Table V-1 provides a brief description of the data being qualified. This information is also provided in Table 4-1.

Table V-1. Data Sources for Qualification within This Work Product

Item	Source	Description of Input Being Qualified	Governing Procedure	Where Used
1	Sunder, S.; Shoesmith, D.W.; and Miller, N.H. 1997. "Oxidation and Dissolution of Nuclear Fuel (UO <sub>2</sub> ) by the Products of the Alpha Radiolysis of Water." <i>Journal of Nuclear Materials</i> , 244, 66-74. Amsterdam, The Netherlands: Elsevier. TIC: 246914 [DIRS143860]	The effects of radiolysis on spent nuclear fuel corrosion (dissolution) will be transitory and will become minor as alpha dose rates decrease.	AP-SIII.9Q Rev. 1/ICN 4	Section 6.2.38; FEP 2.1.13.01.0A
2	Thornton, T.A. 1998. "HPPP Issue 1; Preliminary TSPA for a Pyrophoric Event Involving N-Reactor SNF Waste Packages." Interoffice correspondence from T.A. Thornton (CRWMS M&O) to J.S. Clouet, S.S. Sareen, and D. Stahl, September 21, 1998, LV.WP.TAT.09/98-179, with attachment. MOL.19981019.0001 [DIRS 125082]	Uranium metal-based spent nuclear fuel, particularly the N-Reactor spent nuclear fuel has the potential for pyrophoric behavior.	AP-SIII.2Q Rev 1/ICN 2	Section 6.2.13; FEP 2.1.02.08.0A
3	Rechard, R.P., ed. 1995. Methodology and Results. Volume 2 of Performance Assessment of the Direct Disposal in Unsaturated Tuff of Spent Nuclear Fuel and High-Level Waste Owned by U.S. Department of Energy. SAND94-2563/2. Albuquerque, New Mexico: Sandia National Laboratories. TIC: 237102 [DIRS 101084]	Significant amounts of DSNF cladding are likely to be damaged.	AP-SIII.9Q Rev. 1/ICN 4	Section 6.2.16; FEP 2.1.02.25.0A
4	CRWMS M&O 1997. Waste Package Design Basis Events. BBA000000-01717-0200-00037 REV 00. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19971006.0075 [DIRS 100264]	Maximum allowable waste package interior pressures due to the release of radioactive gases to the interior of the waste package will be too low to compromise waste package integrity.	N/A	Will not be qualified; superceded by BSC 2004 [DIRS 162200]

The information used for direct input is also previously identified in Section 4, and supporting references are clearly identified within Section 6.2, as needed, to provide the technical basis for exclusion of the FEP.

## V.2 THE METHOD OF QUALIFICATION SELECTED AND RATIONALE

The data to be qualified have been extracted from two non-project sources (items 1 and 3) and one product source (item 2). The product source will be qualified by the corroborating data approach outlined in Attachment 3 of AP-SIII.2Q, *Qualification of Unqualified Data*. The data will be qualified for use within this document per Section 5.2.1(1) of AP-SIII.9Q. Per the cited procedure, the corroborating data approach may be used when subject matter data comparisons can be shown to substantiate or confirm parameter values and may include comparisons of unqualified to unqualified data. The use of the corroborative data approach seems most feasible

for judging correctness and reliability by comparing independently developed, but related, data sets.

Other possible qualification methods listed below were reviewed for applicability and will not be used for the following reasons:

- Equivalent QA Program—No QA documentation is available for review. Because of the
  diverse nature and sources of the information used, and because much of the data results
  from primary research activities, it is unlikely that a program equivalency can be
  established or that any available records, practices, or procedures would satisfy YMP
  QA requirements.
- Confirmatory Testing—This testing is not viable because the data relationships and presentations are not amenable to field or laboratory confirmation due to scale, testing resources, and schedule.
- Peer Review–This is not justified because the analysis uses multiple approaches to the problem and there are no critical interpretations of the data.
- Technical Assessment—Technical assessment is not applicable. Most of the cited sources come from peer reviewed journals, or from edited and refereed compendiums of work and, as a result, are assumed a priori to be suitable and reliable with regard to representing the reported work, and there is some attribution of a level of confidence for information from these types of sources. However, because the methods used to acquire the data are only summarily treated in these sources, the documentation or proof of proper data acquisition is unavailable for review.

The procedure allows comparisons of unqualified to unqualified data. In this attachment and Table 6-1, the indirect input information is also referred to as "corroborative/supportive" information to help differentiate it from information being qualified, which is identified as direct input. In some cases, a single source may provide direct and indirect input to the individual FEP analyses in Section 6.2.

## V.3 EVALUATION CRITERIA

The following criteria are established for qualifying these data through corroboration.

- 1. Is there a sufficient quantity of corroborating data available for comparison?
  - Table V-1 is organized by information type to be qualified and lists each of the sources of data to be qualified. For each subject area, at least two independent sources of information were considered for corroboration.
- 2. Can inferences drawn to corroborate these data be clearly identified, justified, and documented?
  - For each source of information to be qualified, the discussion includes a brief statement regarding the original purpose of the study, the method used to acquire the

data, and any limitations germane to the corroborative qualification of the data. Additionally, the basis for assuming adequacy for comparison (e.g. similar type study, update to previous study, compared to previous studies in related fields) will be stated.

For quantitative inputs, corroboration is shown either by graphical representation of the various data sets, or in table or text format, comparing the various values from the various sources.

For qualitative inputs addressing key concepts of a feature, event, or process, one or more corroborative information sources will be used to substantiate the direct input. The source(s) should not conflict with the direct input, and should be in general agreement. This standard may also be used when corroborating boundary conditions that define the conditions necessary for the initiation of a feature, event, or process. For cases with only one available source of information, its appropriateness for use as direct input will be discussed and used only upon mutual agreement of the data qualification team members.

The qualification team consisted of two members: Thomas Thornton, a nuclear fuel expert and the analysis originator (the team chair) and Norman Graves, who is technically competent in radioactive waste management. As the analysis originator, Thornton is not considered to be independent of the information to be qualified (AP-SIII.2Q, Section 5.1.2 (b)(3). However, the procedure requires that the analysis report originator chair the team "...when the qualification is performed within the Analysis or Model Report" (AP-SIII.2Q, Section 5.1.1). Norman Graves did not participate in the acquisition or development of the information, and was, therefore, an independent reviewer of the analysis. The data qualification team considered that the intended use of the data is for FEP screening arguments (for excluded FEPs) and TSPA Disposition discussions (for included FEPs). Therefore, the use of "broad" acceptance criteria is justified, and in lieu of corroboration, a bounding or conservative value (with respect to inclusion of the FEP) may be recommended and considered as qualified under this exercise. Consistent with the intended use, the data qualification team may exercise some latitude in applying these criteria if an adequate explanation or justification for variance from the above criteria can be provided.

For each FEP-specific data set within Section V.2, the evaluation criteria to be applied (i.e., quantitative or qualitative) will be identified.

## V.4 EVALUATION OF THE TECHNICAL CORRECTNESS OF THE DATA

The technical correctness of the data/information used as direct input (and the corroborating information) was evaluated based on the data attributes listed in Attachment 4 of AP-SIII.2Q, *Qualification of Unqualified Data*. Since the information being qualified is qualitative rather than quantitative, planning, collecting, and analyzing the data consisted of identifying the literature sources and assessing the credibility of the corroborating source via the accepted scientific/engineering practice of using the open literature in combination with the team member's technical expertise as shown in sections V.4.x.3. The attributes considered during qualification included:

- 3. The extent to which the data demonstrate the properties of interest (e.g., physical, chemical, geologic, mechanical)
- 7. Prior uses of the data and associated verification processes

- 8. Prior peer or other professional reviews of the data and their results
- 9. Extent and reliability of the documentation associated with the data
- 10. The extent and quality of corroborating data or confirmatory testing results
- 12. The importance of the data to showing that the proposed U.S. Department of Energy repository design meets the performance objectives of 10 CFR 63.

In the data qualification plan, item 2 (technical adequacy of equipment and procedures) was listed as a potentially applicable attribute to be evaluated. However, the technical adequacy of equipment and procedures used to collect and analyze the data was not evaluated due to a general lack of such information in the cited sources.

In the data qualification plan, item 8 (prior peer review) was listed as a potentially applicable attribute to be evaluated. However, the search of the available literature did not disclose any prior peer reviews related to the references to be qualified.

Section V.4 has been subdivided with direct input for each subject FEP being accorded an individual subsection. The discussion of technical correctness for each FEP-specific data set is addressed in four parts.

The first part (Section V.4.x.1) discusses the scope of the literature review. The literature review involved a search of the RIS and the DIRS for the extent of usage in the program, and the number of citations is given in Table V-2 as "relevant use by others."

The second part (Section V.4.x.2) addresses the technical correctness of both the data being qualified, and the corroborating information. Planning, collecting, and analyzing the data consisted of identifying the literature sources and assessing the credibility of the corroborating source via the accepted scientific/engineering practice of using the open literature in combination with the team member's technical expertise. The technical correctness of the data and corroborating information was evaluated based on the attributes listed in Table V-2. This evaluation is presented in table format with attributes 3 through 9, 10, and 12 discussed for the direct inputs and corroborative sources (indirect inputs). In the summary tables, direct input citations are listed in alphabetical order, followed by the corroborative citations. A single cited paper might serve as the source for multiple types of direct input or reference-only information.

By addressing items 2 through 9 for the corroborative information, item 10 is also addressed. However, because the comparison of the direct input to the corroborative information requires more detail, it is specifically addressed in the third part (Section V.4.x.3) for each FEP-specific data set. The discussions for each FEP may be subdivided by topic to facilitate corroboration of the direct inputs.

The fourth part of each section (Section V.4.x.4) provides a recommendation regarding status of the direct input and any associated limitations.

# V.4.1 Data Qualification for Sunder et al. 1997 [DIRS 143860]

The effects of alpha radiolysis could include the production of gas from the waste form and changing the chemistry of the contacting water solutions. The relationship being qualified is stated as:

The effects of radiolysis on spent nuclear fuel corrosion (dissolution) will be transitory and will become minor as dose rates decrease.

#### V.4.1.1 Literature Search

A literature search was performed using the RIS and DIRS databases. Citations from these sources not selected for evaluation were not used if they did not involve waste forms. A pertinent corroborating reference (Gray 1988 [DIRS 168471]) was found that had not been previously used in the main body of this Analysis Report).

## **V.4.1.2** Evaluation of Attributes

For each of the sources to be used in the corroboration of the direct input (Sunder et al. 1997 [DIRS 143860]), the pertinent attributes are summarized in tabular form in Table V-2. These attributes were selected based on a comparison of the pertinent information in the corroborating reference with the reference to be qualified for direct input to the FEPs screening or disposition discussions.

## V.4.1.3 Discussion

The information being qualified is as follows:

Support for the conclusion that the effects of radiolysis on spent nuclear fuel corrosion (dissolution) will be transitory and will become minor as dose rates decrease.

This is the conclusion obtained from the reference cited as direct input (Sunder et al. 1997 [DIRS 143860]). The other reports cited in this discussion are corroborative and support the conclusions of the direct use reference.

Analyses by Sunder and Shoesmith (1991 [DIRS 143815]) and Shoesmith and Sunder (1992 [DIRS 113368]) qualitatively corroborate the information being qualified by showing the waste container will not fail such that water will be shielded from the alpha particles emitted from the fuel. Water will not intrude until gamma and beta emitters (and consequent nitric acid production) have decayed to very low concentrations. In addition, strong gamma and beta fields associated with the used fuel will decrease by a factor of about 1000 in the first few hundred years after disposal.

*In-Package Chemistry for Waste Forms* (BSC 2003 [DIRS 168795], Attachment II) qualitatively corroborates the information being qualified by showing that the degradation of the Zircaloy fuel cladding will not be significantly enhanced by the products of radiolysis. The study also notes:

...the corrosion rate of Zircaloy in water is limited by the slowest of the basic corrosion steps: dissociation of water into oxygen and hydrogen ions, diffusion of oxygen ions through the oxide film, oxidation of the Zr metal, diffusion of electrons through the oxide, and hydrogen-ion reduction by the electrons at the water-to-oxide interface...above about 230°C, diffusion of oxygen ions through the oxide film becomes rate limiting.

If cladding corrosion is controlled by this step, the production of peroxide by radiolysis would have no effect on Zircaloy corrosion even if the alpha dose is higher than expected.

Gray (1988 [DIRS 168471], Summary and Sections 2.0 and 5.1) qualitatively corroborates the information being qualified by providing laboratory test results for leaching of unirradiated  $UO_2$  and spent nuclear fuel. The laboratory experiments indicated that there was little effect due to alpha radiolysis on the leaching behavior of spent nuclear fuel (i.e., with alpha radiation) and  $UO_2$  (without alpha radiation) samples. Most of the difference between the leaching results of the  $UO_2$  and spent nuclear fuel was attributed to surface area difference between them rather than alpha radiolysis per se.

Gamma and Neutron Radiolysis in the 21-PWR Waste Package from Ten to One Million Years (BSC 2002 [DIRS 161912], Sections 6.1, and 6.2) provides justification for screening out neutron and gamma radiolysis by showing nitric acid production to be small at 1,000 years; therefore, it qualitatively corroborates the information being qualified. Gamma and neutron doses decrease respectively by approximately four and two orders of magnitude over the 10,000-year regulatory period. Gamma and Neutron Radiolysis in the 21-PWR Waste Package from Ten to One Million Years (BSC 2002 [DIRS 161912], Section 6.3) further showed that nitric acid production is dominated by gamma production and is insensitive to neutrons. Since the fuel cladding is largely intact, it will isolate water from direct contact with the alpha particles emitted from decay of actinides in the fuel. This provides confidence that radiolysis can be screened out as significantly affecting fuel degradation.

## V.4.1.4 Data Status and Limitations

The conclusion by Sunder et al. (1997 [DIRS 143860]) that the effect of radiolysis on spent nuclear fuel corrosion (dissolution) will be transitory and will become minor as dose rates decrease is qualified for its intended use in this product. Sunder et al. (1997 [DIRS 143860]) as an outside-the-project source may be regarded as qualified (per AP-SIII.9Q) for use in this analysis report because it is a report in *Journal of Nuclear Materials*, a highly reputable and peer-reviewed technical publication (reliability of data source, and the availability of the corroborating data). The discussion in Section V.4.1.3 qualitatively substantiated this conclusion. There is no limit on the data use in this anlysis report.

# V.4.2 Data Qualification for Thornton 1998 [DIRS 125082]

## V.4.2.1 Literature Search

The literature search identified an additional pertinent corroborating reference that was not included in the main body of the analysis report for the qualification of Thornton (1998 [DIRS 125082] in Swanson et al. (1985 [DIRS 168468]).

#### V.4.2.2 Evaluation of Attributes

Table V-2 summarizes pertinent attributes for each of the sources used to corroborate the direct input (Thornton 1998 [DIRS 125082]). These attributes were selected based on comparing the pertinent corroborating reference information in the corroborating reference to the reference to be qualified for direct input to the FEPs screening or disposition discussions.

#### V.4.2.3 Discussion

The information being qualified is that:

Uranium metal-based spent nuclear fuel, particularly the N-Reactor spent nuclear fuel, has the potential for pyrophoric behavior.

This is the conclusion obtained from the reference cited as direct input (Thornton 1998 [DIRS 125082]). The other reports cited in this discussion/analysis are corroborative, and support he conclusions of the direct use reference.

Schulz (1972 [DIRS 159406]) qualitatively corroborates the information being qualified by analyzing several unanticipated pyrophoric events that occurred during N-Reactor fuel reprocessing at the West Valley reprocessing facility (circa 1967-1968). These uranium metal fires occurred primarily as a result of the aggressive mechanical handling of the fuel elements during discharge from the N-Reactor (at Hanford), subsequent transport to West Valley (New York) in water-filled casks, and loading into the reprocessing dissolver vessels. The fuel often sustained damage sufficient to breach the Zircaloy cladding because reactor discharge involved pushing the elements from an approximately 15-foot drop into a collector basket. consequent exposure of the chemically active uranium metal that comprised the core of the fuel elements made it susceptible to further corrosion and damage. When loaded and processed in the dissolvers, the resulting material became susceptible to ignition and burning. Nineteen dissolver pyrophoric events (fires) occurred between 1967 and 1968. Fourteen fires occurred inside the dissolvers, four in the bins into which the Zircoloy "hulls" were dumped after the dissolution operation, and one on the canyon deck after a hull fell on it. During these reactor discharge, transport, and reprocessing operations, the N-Reactor fuel element metallic uranium cores were exposed to air and water, thus exposing the chemically active uranium metal surfaces to a strong oxidizing environment. It was surmised that sparks resulting from element-to-element contact provided the ignition source and that the materials that initially ignited were weld beads sensitized by exposure to the highly acidic environment in the dissolvers.

Swanson et al. (1985 [DIRS 168468]) qualitatively corroborates the information being qualified by providing an independent analysis and alternative explanation for the N-Reactor SNF

pyrophoric events that occurred in the dissolvers at the West Valley reprocessing plant. They concluded that the material that initially ignited was the metallic uranium, or more particularly the uranium hydride inclusions (resulting from corrosion) embedded in the uranium metal.

Abrefah et al. (1995 [DIRS 151125]) qualitatively corroborate the information being qualified by reporting the results of visual examinations of N-Reactor SNF elements that underwent characterization in support of the development of a dry intermediate storage facility at Hanford. It was evident that a significant fraction of the N-Reactor spent fuel is currently damaged, and so will be damaged at the time of emplacement in the repository. The potential for ignition and subsequent burning of the uranium metal would be expected to be proportional to the amount of exposed and corroded uranium metal and therefore on the fraction of N-Reactor spent nuclear fuel assemblies having breached cladding. Taken together with the Schulz (1972 [DIRS 159406]) analyses of the N-Reactor fuel ignition at West Valley, the observation of extensive damaged cladding indicates that the current condition of the N-Reactor spent nuclear fuel makes it potentially pyrophoric.

Abrefah et al. (1999 [DIRS 151226] and Marschman et al. (1997 [DIRS 149429) qualitatively corroborate the information being qualified by identifying uranium hydride inclusions in the exposed uranium metal surfaces. Uranium hydride is suspected of being the potential source of pyrophoric behavior in uranium metal that has corroded in the air or water environment.

Thornton (1998 [DIRS 125082]) makes the overall case that pyrophoric behavior in metallic uranium and uranium metal-based spent nuclear fuel is possible in an oxidizing environment (air or water) and under conditions of mechanical trauma. This environment is not expected while the waste packages and canisters remain intact, but could occur after waste package failure. Attachment I justifies the conclusion that even in the event a pyrophoric event occurs after waste package failure, the effect on the boundary dose will be minor.

#### V.4.2.4 Data Status and Limitations

Neither "HPPP Issue 1; Preliminary TSPA for a Pyrophoric Event Involving N-Reactor SNF Waste Packages" (Thornton 1998 [DIRS 125082]) nor its corroborating information enable a direct estimate of the precise conditions under which pyrophoric behavior would occur. They also do not provide direct answers to questions such as: "At what temperature will a damaged N-Reactor fuel assembly ignite," or, "How hard an impact from an accidental drop of an open canister containing damaged N-Reactor fuel elements can be tolerated?" *Standard Guide for Pyrophoricity/Combustibility Testing in Support of Pyrophoricity Analyses of Metallic Uranium Spent Nuclear Fuel* (ASTM C 1454-00 [DIRS 152779]) provides further guidance in this area. However, for the purposes of this analysis report, such estimates are unnecessary since the screening decision to exclude DSNF cladding (Section 6.2.13) and the consequence analysis (Attachment I) assume a pyrophoric event will occur when a waste package containing N-Reactor SNF fails. Therefore, "HPPP Issue 1; Preliminary TSPA for a Pyrophoric Event Involving N-Reactor SNF Waste Packages" (Thornton 1998 [DIRS 125082]) should be regarded as qualified for its use in Section 6.2.13.

# V.4.3 Data Qualification for Rechard 1995 [DIRS 101084]

## V.4.3.1 Literature Search

The literature search identified an additional pertinent corroborating reference (Lawrence 1999 [DIRS 168475]) not included in the analysis report for the qualification of *Methodology and Results* (Rechard 1995 [DIRS 101084]).

#### V.4.3.2 Evaluation of Attributes

For each of the sources to be used in the corroboration of the direct input (Rechard 1995 [DIRS 101084]), the pertinent attributes are summarized in tabular form in Table V-2. These attributes were selected based on comparing the pertinent information in the corroborating reference with the reference to be qualified for direct input to the FEPs screening or disposition discussions.

## V.4.3.3 Discussion

The information being qualified is:

Significant amounts of DSNF cladding are likely to be damaged.

This is the conclusion obtained from the reference cited as direct input (Rechard 1995 [DIRS 101084]). The other reports cited in this discussion are corroborative and support the conclusions of the direct use reference.

Abrefah et al. (1995 [DIRS 151125]) characterized samples of the N-Reactor spent fuel stored in the K-East and K-West basins on the Hanford site. N-Reactor fuel consists of cylinders of uranium metal clad in Zircaloy. This work was done in support of the plan to remove the N-Reactor SNF from the K-East and K-West pools. This included drying the SNF, putting it in sealed and helium-inerted canisters (called MCOs or multi-canister overpacks), and placing them in dry interim storage at the Hanford site pending ultimate disposal at Yucca Mountain. This characterization revealed a significant (but not fully quantified) fraction of the cladding had been damaged. In addition, reaction of the exposed uranium with the water in the K-basins had resulted in the formation of uranium hydride inclusions in the exposed uranium. As discussed in Section 6.2.13 and Attachment I, these uranium hydride inclusions are considered conditions supporting pyrophoric behavior in uranium and uranium metal-based SNF.

DSNF and Other Waste Form Degradation Abstraction (BSC 2003 [DIRS 163693]) discusses the grouping of the many types DSNF (see Section 6.2.17). The report notes that few groups have had their cladding characterized enough to take credit for intact cladding in their performance analyses. Additionally, it notes that the N-Reactor SNF constitutes over 80 percent by weight of the total DSNF. The report suggests that no credit should be taken for DSNF cladding in the TSPA because the status of the majority of the DSNF groups is unknown and a significant fraction of the N-Reactor SNF has damaged or perforated cladding.

Lawrence (1999 [DIRS 168475], Section 5.1 and Table 1) reports on the results of an effort to estimate the fraction of perforated N-Reactor SNF cladding. The perforation types were

described as breached (minor cladding rupture), defected (significant uranium metal exposed), or bad (gross failure). The identification of perforated elements and their categorization was done by means of either a visual or a video examination of 200 fuel elements from each of the K-East and K-West basins. The examination showed 65 (32.5 percent–18 breached, 42 defected, and 5 bad) K-East basin elements and 66 (33 percent–53 breached, 0 defected, and 13 bad) K-West basin elements were perforated.

Each of these references shows that the degree of cladding damage to the N-Reactor SNF is significant. Additionally, there is an unquantified uncertainty in the estimates of cladding failure due to the relatively inexact nature of the visual observations. The information in these references sufficiently resembles the estimates of failed fuel by Rechard (1995 [DIRS 101084]) to support the conservative decision to take no credit for radionuclide retardation by the DSNF cladding in the TSPA.

Rechard (1995 [DIRS 101084]) as an outside-the-project source may be regarded as qualified (per AP-SIII.9Q) for use in this analysis report because it is generated at Sandia National Laboratory, and is thereby a reputable and peer-reviewed technical publication (reliability of data source), and the availability of the corroborating data in the other sources.

## V.4.3.4 Data Status and Limitations

The N-Reactor SNF characterization reported by Abrefah et al. (1995 [DIRS 151125]) was obtained from fuel elements known to be defected. The results of the optical metallographic examinations (e.g., identifying uranium hydride inclusions in the corroded uranium surfaces) agreed qualitatively with other available information. However, these results could not be used to estimate the fraction of failed fuel elements. In addition, these studies did not provide information to predict or to estimate the extent of further cladding damage during interim storage at Hanford and transport to the repository. However, this uncertainty further supports the decision to take no credit for the DSNF cladding in TSPA. Since information provided by Rechard (1995 [DIRS 101084]) was used to justify not taking credit for any DSNF cladding in the TSPA, this reference may be regarded as qualified for its use in Section 6.2.16.

Table V-2. Sources and Attributes Evaluation for Direct Inputs

ion Extent and is Reliability of Documentation	Moderate to High –	Moderate
Qualification Attributes Addressed	3, 9, 10	3, 10
Relevant Use by Others	ANL-EBS-MD-000037, REV 03 000-30R-EBS0-00100-000-000	ANL-WIS-MD-000009, REV 00 ICN 01
Corroborating References	BSC (Bechtel SAIC Company) 2002. Gamma and Neutron Radiolysis in the 21-PWR Waste Package from Ten to One Million Years. 000-00C-DSU0-00700-000-00A. Las Vegas, Nevada: Bechtel SAIC Company. ACC: MOL.20021004.0002 [DIRS 161912] Section 6.3 and Figure 5	Sunder, S. and Shoesmith, D.W. 1991. Chemistry of UO <sub>2</sub> Fuel Dissolution in Relation to the Disposal of Used Nuclear Fuel. AECL-10395. Pinawa, Manitoba, Canada: Whiteshell Laboratories, Atomic Energy of Canada Limited. TIC: 246920
Direct Input Usage	Section 6.2.38 (FEP 2.1.13.01.0A) Support for the conclusion that the effects of alpha radiolysis on spent fuel corrosion (dissolution) will be transitory and will become minor as alpha dose rates decrease.	
Source to be Qualified	Sunder, S.; Shoesmith, D.W.; and Miller, N.H. 1997. "Oxidation and Dissolution of Nuclear Fuel (UO <sub>2</sub> ) by the Products of the Alpha Radiolysis of Water." <i>Journal of Nuclear Materials</i> , 244, 66-74. Amsterdam, The Netherlands: Elsevier. TIC: 246914 [DIRS 143860]	
Item	-	

ANL-WIS-MD-000009 REV 01

Table V-2. Sources and Attributes Evaluation for Direct Inputs (Continued)

					Qualification	Extent and
			Corroborating		Attributes	Reliability of
Item	Source to be Qualified	Direct Input Usage	References	Relevant Use by Others	Addressed	Documentation
			Shoesmith, D.W. and	ANL-EBS-MD-000015 REV 01	3, 10	Moderate
			Sunder, S. 1992. "The	ICN 01		
			Prediction of Nuclear Fuel			
			(UO2) Dissolution Rates	ANL-EBS-MD-000019		
			Under Waste Disposal	REV 00 CN 01		
			Conditions." Journal of			
			Nuclear Materials, 190, 20-			
			35. Amsterdam, The			
			Netherlands: Elsevier.			
			TIC: 246431 [DIRS			
			113368]			
			BSC (Bechtel SAIC	ANL-EBS-GS-000001, REV 00	3,7,9,10,12	High
			Company) 2003. Errata	ANL-EBS-PA-000007, REV 00		
			for In-Package Chemistry	CAL-EBS-MD-000020, REV 00		
			for Waste Forms. ANL-	CAL-EBS-PA-000005, REV 00		
			EBS-MD-000056 REV 00.	MDL-DSU-MD-000001, REV 00		
			Las Vegas, Nevada:			
			Bechtel SAIC Company.			
			ACC:			
			MOL.20010322.0490;			
			DOC.20031014.0005.			
			[DIRS 168795]			

ANL-WIS-MD-000009 REV 01

Table V-2. Sources and Attributes Evaluation for Direct Inputs (Continued)

Item	Source to be Qualified	Direct Input Usage	Corroborating References	Relevant Use by Others	Qualification Attributes Addressed	Extent and Reliability of Documentation
			Gray, W.J. 1988. Effect of Surface Oxidation, Alpha Radiolysis, and Salt Brine Composition on Spent Fuel and UO <sub>2</sub> Leaching Performance. PNL/SRP/6689 HQX.19881021.0025 Summary and Section 5.1.[DIRS 168471] (This reference is not used in the body of the report.)	N/A	3, 10	Moderate-to- Low
Ν	Thornton, T.A. 1998. "HPPP Issue 1; Preliminary TSPA for a Pyrophoric Event Involving N-Reactor SNF Waste Packages." Interoffice correspondence from T.A. Thornton (CRWMS M&O) to J.S. Clouet, S.S. Sareen, and D. Stahl, September 21, 1998, LV.WP.TAT.09/98-179, with attachment. MOL.19981019.0001	Section 6.2.13 (FEP 2.1.02.08.0A) Provides analyses and examples of the potential for pyrophoric behavior in uranium metalbased spent fuel, particularly the N-Reactor spent fuel.	Schulz, W.W. 1972. Shear-Leach Processing of N-Reactor Fuel Cladding Fires. ARH-2351. Richland, Washington: Atlantic Richfield Hanford. TIC: 243079. [DIRS 159406] (pyrophoric behavior of N-Reactor SNF at West Valley)	ANL-WIS-MD-000004 REV 02	3, 10	Moderate-to- Low

ANL-WIS-MD-000009 REV 01

**April** 2004

Miscellaneous Waste Form FEPs: Data Qualification

Table V-2. Sources and Attributes Evaluation for Direct Inputs (Continued)

					Qualification	Extent and
			Corroborating		Attributes	Reliability of
Item	Source to be Qualified	Direct Input Usage	References	Relevant Use by Others	Addressed	Documentation
			Abrefah, J.; Gray, W.J.;	ANL-WIS-MD-000004 REV 02	9, 10	Moderate-to-
			Ketner, G.L.; Marschman,	ICN 01		High
			S.C.; Pyecha, T.D.; and			
			Thornton, T.A. 1995. K-			
			Basin Spent Nuclear Fuel			
			Characterization Data			
			Report. PNL-10778.			
			Richland, Washington:			
			Pacific Northwest National			
			Laboratory. TIC: 243197.			
			[DIRS 151125]			
			(extensive N-Reactor			
			SNFcladding damage)			
			Abrefah, J.; Huang, F.H.;	ANL-WIS-MD-000004 REV 02	3, 9, 10	Moderate-to-
			Gerry, W.M.; Gray, W.J.;	ICN 01		High
			Marschman, S.C.; and			
			Thornton, T.A. 1999.			
			Analysis of Ignition Testing			
			on K-West Basin Fuel.			
			PNNL-11816. Richland,			
			Washington: Pacific			
			Northwest National			
			Laboratory. TIC: 248558.			
			[DIRS 151226]			
			(hydrides concentrate near			
			exposed U metal surfaces)			

ANL-WIS-MD-000009 REV 01

Table V-2. Sources and Attributes Evaluation for Direct Inputs (Continued)

	2000	Relevant Use by Others	Addressed	
	Marschman, S.C.; Pyecha, T.D.; and Abrefah, J. 1997.	ANL-WIS-MD-000004 REV 02 ICN 01	9, 10	Moderate-to- High
	Metallographic			)
	Examination of Damaged			
	N Reactor Spent Nuclear			
	Fuel Element			
	SFEC5,4378. PNNL-			
	11438. Richland,			
	Washington: Pacific			
	Northwest National			
	Laboratory. TIC: 248059.			
	[DIRS 149429]			
	Swanson, J.L.; Bray, L.A	N/A	3, 9, 10	Moderate
	Kjarmo, H.E.; Ryan, J.L.;			
	Matsuzaki, C.L.; Pitman,			
	S.G.; and Haberman, J.H.			
	1985. Laboratory Studies			
	of Shear/Leach Processing			
	of Zircaloy Clad Metallic			
	Uranium Reactor Fuel.			
	PNL-5708. Richland,			
	Washington: Pacific			
	Northwest Laboratory.			
	ACC:MOL.20040325.0049			
	[DIRS 168468]			
	(Pyrophoricity in damaged			
	N-Reactor SNF)			
	(this reference is not cited			
	in the main body of this			
	report)			

V-17 of V-22 April 2004

ANL-WIS-MD-000009 REV 01

Table V-2. Sources and Attributes Evaluation for Direct Inputs (Continued)

ANL-WIS-MD-000009 REV 01

**April** 2004

Table V-2. Sources and Attributes Evaluation for Direct Inputs (Continued)

			Corroborating		Qualification Attributes	Extent and Reliability of
Item	Source to be Qualified	Direct Input Usage	References	Relevant Use by Others	Addressed	Documentation
			Lawrence, L.A., 1999. <i>K</i>	N/A	3, 10	Moderate
			Basin Spent Nuclear Fuel			
			Characterization. HNF-			
			3534, Rev. 0. Richland,			
			Washington: Duke			
			Engineering & Services			
			Hanford.			
			ACC:MOL.20040325.0053			
			[DIRS 168475], Section			
			5.1 and Table 1)			
			(estimate of the fraction of			
			failed N-reactor SNF from			
			the K-East and K-West			
			spent fuel pools)			

ANL-WIS-MD-000009 REV 01

April 2004

#### V.5 DATA GENERATED BY THE EVALUATION

No data was generated by this qualification effort. Analyses were performed as shown herein to allow corroboration of direct input to indirect inputs. However, the results of the analyses are not being qualified and are not to be used directly as data or serve as the sole basis for FEP screening decisions.

#### V.6 THE EVALUATION RESULTS

The third section for each FEP data set (Section V.4.x.3) provides a comparison of the data being qualified to the corroborative information. Any necessary manipulations or calculations for the comparison are provided in that section of the discussion. In some case, this may be further subdivided by specific data topic.

# V.7 CONCLUSION FOR/AGAINST CHANGING THE QUALIFICATION STATUS

This is addressed in Section V.4.x.4 for each FEP-specific data set. The fourth section of the discussion for each FEP data set provides a statement of recommendation and a discussion of any specific limitations that apply. This is addressed for each FEP-specific data set under the heading "Data Status and Limitation."

The direct inputs listed and discussed above have been reviewed against the stated review criteria. In some cases, limitations have been applied. However, all the data evaluated satisfied the respective criteria and the status should be changed from "unqualified" to "qualified."

# V.8 RATIONALE FOR ABANDONING ANY OF THE QUALIFICATION METHODS

This section is not applicable. All three of the references are qualified using corroboration. The basis for not selecting other qualification methods is previously discussed in Section 1.2.

#### V.9 LIMITS OR CAVEATS

The intended use of the data qualified here is for use in FEP screening. For all data discussed in Section V.2, the data provide a desired level of confidence that is suitable for the intended use. The data are being qualified within this technical product only for this work product and should not be used or referenced by others as direct input without qualification external to this technical product. The fourth section of the discussion for each FEP data set specifies any additional applicable limitations. This is addressed for each FEP-specific data set under the heading "Data Status and Limitation."

# V.10 IDENTIFICATION OF ANY SUPPORTING INFORMATION

Supporting information (i.e. corroborating information) is identified in Section V.4.x.2 of each FEP-specific data set. The table includes an appropriate reference identifier for each citation, such as an accession number, DIRS number, or Technical Information Center catalog number.

### V.11 DATA QUALIFICATION PLAN

The data qualification activities documented herein are outlined in the data qualification plan (Attachment VI).

Deviations from the data qualification plan implemented during its execution include the following:

- Waste Package Design Basis Events (CRWMS M&O 1997 [DIRS 100264]) was not qualified per the plan because in the interim a better reference (BSC 2004 [DIRS 162200]) was found to support the screening argument in Section 6.2.37.
- Items 1 and 3, being data obtained from outside sources, were additionally qualified to the requirements of AP-SIII.9Q Rev.1/ICN 4 for qualifying outside source data.
- Attribute 2 was not used.
- Attribute 8 was listed in the Data Qualification Plan (Attachment VI) as being invoked, but was not used in this Data Qualification Report.
- Rev. 1, ICN 3 of AP-SIII.9Q, *Scientific Analyses*, was identified in the Data Qualification Plan (Attachment VI) as the governing procedure for Scientific Analyses. It has since been superseded by Rev. 1, ICN 4.
- On the cover of the Data Qualification Plan, Section 5.3.2 was identified as the section of AP-SIII.2Q covering documentation. The correct section is 5.3.1.

Miscellaneous Waste Form FEPs: Data Qualification

INTENTIONALLY LEFT BLANK

# ATTACHMENT VI – DATA QUALIFICATION PLAN (SCANNED IMAGES)

500		D	QA: QA
BSC		DATA QUALIFICATION PLAN	Page 1 of 1
Section I. Organization	anal Information		
Qualification Title	mar information		
Waste Form FEPs Data C	Qualification		
Requesting Organization			
EBS			
Section II. Process P	lanning Requirem	nents	
List of Unqualified Data to	be Evaluated		
The data to be qualified a DIRS numbers are provid been obtained and entered	ed. Sources that do	eginning on page 1 of the attachment to this data qualificent not have TIC or DIRS numbers listed will have these nursy system.	ication plan. Available TIC and/or umbers assigned when they have
		ationale for selection of method(s) (Attachment 3) and qualifica ualified by corroboration as discussed on page 1 of the a	
3. Data Qualification Team a	and Additional Support S	Staff Required	
Qualification Chairperson Thomas Thornton, - Technically Competent Ir Norman Graves – PA QA Representation This qualification task qualification team	PA – EBS ndividual (s). TSPA	A Program equivalency; therefore, a representative of BS	SC QA is not included on the data
Data Evaluation Criteria			
	are specified starting	g on Page 2 of the attachment to this data qualification p	lan.
· · · · · · · · · · · · · · · · · · ·			
5. Identification of Procedure	es Used	43 °	
Technical Product, ANL-	WIS-MD-000009 RE	ation effort is AP-SIII.2Q REV 1 ICN 2. Data qualification V 01, Miscellaneous Waste-Form FEPs, per Section 5.3. roduct is AP-SIII.9Q REV 1 ICN 3.	n will be documented in the 2 of AP-SIII.2Q REV 1 ICN 2.
Seed III A	<u>, j</u>		
Section III. Approval			15.4
Qualification Chairpersor	Printed Name	Qualification Chairperson Signature	Date 3/2 4/004
Thomas Thornton ,	inted None	Parasilla Manda Sir Lite	Data
Responsible Manager Pr Howard Adkins	inted iname	Responsible Manager Signature	7/24/04 Date 03-24-04
I IOWalu Aukilis		Kully C. Mic	01 07

PA\_ASIII2-1 (Rev. 01/29/2004)

D00	DATA QUALIFICATION PLAN	QA: QA
BSC	ATTACHMENT	Page 1 of 3

#### Table 1 Data To Be Qualified

Item	Source	Description	AMR Section
1	Sunder, S.; Shoesmith, D.W.; and Miller, N.H. 1997. "Oxidation and Dissolution of Nuclear Fuel (UO <sub>2</sub> ) by the Products of the Alpha Radiolysis of Water." <i>Journal of Nuclear Materials</i> , 244, 66-74. Amsterdam, The Netherlands: Elsevier. TIC: 246914 [DIRS143860]	Support for the conclusion that the effects of alpha radiolysis on spent fuel corrosion (dissolution) will be transitory and will become minor as alpha dose rates decrease	Section 6.2.38
2	Thornton, T.A. 1998. "HPPP Issue 1; Preliminary TSPA for a Pyrophoric Event Involving N-Reactor SNF Waste Packages." Interoffice correspondence from T.A. Thornton (CRWMS M&O) to J.S. Clouet, S.S. Sareen, and D. Stahl, September 21, 1998, LV.WP.TAT.09/98-179, with attachment. MOL.19981019.0001 [DIRS 125082]	Provides analyses and examples of the potential for pyrophoric behavior in uranium metal-based spent fuel, particularly the N-reactor spent fuel.	Section 6.2.13
3	Rechard, R.P., ed. 1995. Methodology and Results. Volume 2 of Performance Assessment of the Direct Disposal in Unsaturated Tuff of Spent Nuclear Fuel and High-Level Waste Owned by U.S. Department of Energy. SAND94-2563/2. Albuquerque, New Mexico: Sandia National Laboratories. TIC: 237102	Estimate of the amount of damaged cladding in DSNF. For approximately 80% of the DSNF that is N-Reactor SNF, the cladding will be significantly damaged at the time of emplacement in their canisters. Up to 50 percent may be already perforated.	Section 6.2.16
4	CRWMS M&O 1997. Waste Package Design Basis Events. BBA000000-01717-0200-00037 REV 00. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19971006.0075 [DIRS 100264]	Maximum allowable waste package interior pressures due to the release of radioactive gases to the interior of the waste package will be too low to compromise waste package integrity.	Section 6.2.37

#### DATA QUALIFICATION METHOD

The direct inputs from non-YMP sources used for the Miscellaneous Waste Form FEPs analyses will be qualified in accordance with the requirements of Method 2, *Corroborating Data*, of Attachment 3 to AP-SIII.2Q, *Qualification Of Unqualified Data*.

The qualification methods of Equivalent QA Programs, Confirmatory Testing, Peer Review, and Technical Assessment were reviewed for applicability and will not be utilized.

- Equivalent QA Program The single journal article to be qualified was developed external to OCRWM. It would be far to expensive and time consuming to identify and evaluate QA practices, if any, that were employed in producing this document. The remaining documents were produced as non-Q documents under OCRWM funded activities.
- Confirmatory Testing Confirmatory testing is not amenable to field or laboratory confirmation due to scale, testing resources, and schedule.
- Peer Review Peer review is not justified because the analysis uses multiple approaches to the problem, and there are no critical interpretations of the data.
- Technical Assessment Technical Assessment will not be used primarily because all of the data to be qualified can be independently corroborated.

The approach that seems most feasible for judging correctness and reliability is that of comparing independently developed, but related, data sets (Corroborative Data).

Per the cited procedure (AP-SIII.2Q Rev 1 ICN 2), the Corroborating Data approach may be used when subject matter data comparisons can be shown to substantiate or confirm parameter values and may include

PA ASIII2-1 (Rev. 01/29/2004)

	DATA QUALIFICATION PLAN	QA: QA
BSC	ATTACHMENT	Page 2 of 3

comparisons of unqualified to unqualified data. Where the information is available, data attributes from Attachment 4 of AP-SIII.2Q that will be considered during qualification include:

- 2. The technical adequacy of equipment and procedures used to collect and analyze the data.
- 3. The extent to which the data demonstrate the properties of interest (e.g., physical, chemical, geologic, mechanical).
- 7. Prior uses of the data and associated verification processes.
- 8. Prior peer or other professional reviews of the data and their results.
- 9. Extent and reliability of the documentation associated with the data.
- 10. The extent and quality of corroborating data or confirmatory testing results
- 12. The importance of the data to showing that the proposed U.S. Department of Energy repository design meets the performance objectives of 10 CFR 63."

It is the intent of this data qualification effort that comparison of the various unqualified data sets be used to qualify the direct inputs within the technical work product. Data sets used as direct input are listed above and will be qualified. Corroborating data are indirect input, which will not be qualified and are not listed above. Corroborating data will be clearly identified in the qualification documentation provided in the technical product consistent with the requirements of AP-SIII.9Q.

#### DATA EVALUATION CRITERIA

The following criteria are established for qualifying these data through corroboration.

- 1. Is there a sufficient quantity of corroborating data available for comparison?
  - The above table is organized by type of information to be qualified, and each of the sources of data to be qualified is listed. For each subject area at least two, and preferably three or more, independent sources of data will be considered.
- 2. Can inferences drawn to corroborate these data be clearly identified, justified, and documented?
  - For each source of information to be qualified, the discussion will include a brief statement regarding the original purpose of the study, the method used to acquire the data, and any limitations germane to the corroborative qualification of the data. Additionally, the basis for assuming adequacy for comparison (e.g. similar type study, update to previous study, compared to previous studies in related fields) will be stated.

For quantitative inputs, corroboration will be shown either by graphical representation of the various data sets, or in table or text format, comparing the various values from the various sources. Corroboration will be considered acceptable, if "singular" are shown to be within 2 standard deviations of the mean value, with the mean and deviations developed by equal weighting of reported mean values from each source. In the case of probability distributions or equations based on probability distributions corroboration will be considered acceptable if the resulting probability distributions fall within 2 orders of magnitude for any given point in the distribution.

For qualitative inputs addressing key concepts of a feature, event, or process, one or more corroborative information sources will be used to substantiate the direct input. The source(s) should not conflict with the direct input, and should be in general agreement. This standard may also be used when corroborating boundary

PA\_ASIII2-1 (Rev. 01/29/2004)

BSC

DATA QUALIFICATION PLAN
ATTACHMENT

QA: QA
Page 3 of 3

conditions that define the conditions necessary for the initiation of a feature, event, or process (e.g., temperature and pressure conditions associated with metamorphism). For cases with only one available source of information, the appropriateness for use as direct input will be discussed, and the direct input utilized only upon mutual agreement of the data qualification team members.

The data qualification team will consider that the intended use of the data is for FEPs screening. Therefore, the use of "broad" acceptance criteria is justified, and in lieu of corroboration, a bounding or conservative value (with respect to inclusion of the FEP) may be recommended and considered as qualified under this exercise. Consistent with the intended use, the data qualification team may exercise some latitude in applying these criteria if an adequate explanation or justification for variance from the above criteria can be provided.

PA\_ASIII2-1 (Rev. 01/29/2004)